Part IB — Statistics

Based on lectures by D. Spiegelhalter

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These notes are not endorsed by the lecturers, and I have modified them (often significantly) after lectures. They are nowhere near accurate representations of what was actually lectured, and in particular, all errors are almost surely mine.

Estimation
Review of distribution and density functions, parametric families. Examples: binomial, Poisson, gamma. Sufficiency, minimal sufficiency, the Rao-Blackwell theorem. Maximum likelihood estimation. Confidence intervals. Use of prior distributions and Bayesian inference. [5]

Hypothesis testing
Simple examples of hypothesis testing, null and alternative hypothesis, critical region, size, power, type I and type II errors, Neyman-Pearson lemma. Significance level of outcome. Uniformly most powerful tests. Likelihood ratio, and use of generalised likelihood ratio to construct test statistics for composite hypotheses. Examples, including t-tests and F-tests. Relationship with confidence intervals. Goodness-of-fit tests and contingency tables. [4]

Linear models
Derivation and joint distribution of maximum likelihood estimators, least squares, Gauss-Markov theorem. Testing hypotheses, geometric interpretation. Examples, including simple linear regression and one-way analysis of variance. Use of software. [7]

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0 Introduction

Statistics is a set of principles and procedures for gaining and processing quantitative evidence in order to help us make judgements and decisions. In this course, we focus on formal *statistical inference*. In the process, we assume that we have some data generated from some unknown probability model, and we aim to use the data to learn about certain properties of the underlying probability model.

In particular, we perform *parametric inference*. We assume that we have a random variable X that follows a particular known family of distribution (e.g. Poisson distribution). However, we do not know the parameters of the distribution. We then attempt to estimate the parameter from the data given.

For example, we might know that $X \sim \text{Poisson}(\mu)$ for some μ, and we want to figure out what μ is.

Usually we repeat the experiment (or observation) many times. Hence we will have $X_1, X_2, \cdots, X_n$ being iid with the same distribution as X. We call the set $\mathbf{X} = (X_1, X_2, \cdots, X_n)$ a *simple random sample*. This is the data we have.

We will use the observed $\mathbf{X} = \mathbf{x}$ to make inferences about the parameter θ, such as

- giving an estimate $\hat{\theta}(\mathbf{x})$ of the true value of θ.
- Giving an interval estimate $(\hat{\theta}_1(\mathbf{x}), \hat{\theta}_2(\mathbf{x}))$ for θ
- testing a hypothesis about θ, e.g. whether $\theta = 0$.

1 Estimation

1.1 Estimators

The goal of estimation is as follows: we are given iid $X_1, \cdots, X_n$, and we know that their probability density/mass function is $f_X(x; \theta)$ for some unknown θ. We know f_X but not θ. For example, we might know that they follow a Poisson distribution, but we do not know what the mean is. The objective is to estimate the value of θ.

Definition (Statistic)**.** A *statistic* is an estimate of θ. It is a function T of the data. If we write the data as $\mathbf{x} = (x_1, \cdots, x_n)$, then our estimate is written as $\hat{\theta} = T(\mathbf{x})$. $T(\mathbf{X})$ is an *estimator* of θ.

The distribution of $T = T(\mathbf{X})$ is the *sampling distribution* of the statistic.

Note that we adopt the convention where capital $\mathbf{X}$ denotes a random variable and $\mathbf{x}$ is an observed value. So $T(\mathbf{X})$ is a random variable and $T(\mathbf{x})$ is a particular value we obtain after experiments.

Example. Let $X_1, \cdots, X_n$ be iid $N(\mu, 1)$. A possible estimator for μ is

$$T(\mathbf{X}) = \frac{1}{n}\sum X_i.$$

Then for any particular observed sample $\mathbf{x}$, our estimate is

$$T(\mathbf{x}) = \frac{1}{n}\sum x_i.$$

What is the sampling distribution of T? Recall from IA Probability that in general, if $X_i \sim N(\mu_i, \sigma_i^2)$, then $\sum X_i \sim N(\sum \mu_i, \sum \sigma_i^2)$, which is something we can prove by considering moment-generating functions.

So we have $T(\mathbf{X}) \sim N(\mu, 1/n)$. Note that by the Central Limit Theorem, even if X_i were not normal, we still have approximately $T(\mathbf{X}) \sim N(\mu, 1/n)$ for large values of n, but here we get exactly the normal distribution even for small values of n.

The estimator $\frac{1}{n}\sum X_i$ we had above is a rather sensible estimator. Of course, we can also have silly estimators such as $T(\mathbf{X}) = X_1$, or even $T(\mathbf{X}) = 0.32$ always.

One way to decide if an estimator is silly is to look at its *bias*.

Definition (Bias)**.** Let $\hat{\theta} = T(\mathbf{X})$ be an estimator of θ. The *bias* of $\hat{\theta}$ is the difference between its expected value and true value.

$$\text{bias}(\hat{\theta}) = \mathbb{E}_\theta(\hat{\theta}) - \theta.$$

Note that the subscript $_\theta$ does not represent the random variable, but the thing we want to estimate. This is inconsistent with the use for, say, the probability mass function.

An estimator is *unbiased* if it has no bias, i.e. $\mathbb{E}_\theta(\hat{\theta}) = \theta$.

To find out $\mathbb{E}_\theta(T)$, we can either find the distribution of T and find its expected value, or evaluate T as a function of $\mathbf{X}$ directly, and find its expected value.

Example. In the above example, $\mathbb{E}_\mu(T) = \mu$. So T is unbiased for μ.

1.2 Mean squared error

Given an estimator, we want to know how good the estimator is. We have just come up with the concept of the *bias* above. However, this is generally not a good measure of how good the estimator is.

For example, if we do 1000 random trials $X_1, \cdots, X_{1000}$, we can pick our estimator as $T(\mathbf{X}) = X_1$. This is an unbiased estimator, but is really bad because we have just wasted the data from the other 999 trials. On the other hand, $T'(\mathbf{X}) = 0.01 + \frac{1}{1000}\sum X_i$ is biased (with a bias of 0.01), but is in general much more trustworthy than T. In fact, at the end of the section, we will construct cases where the only possible unbiased estimator is a completely silly estimator to use.

Instead, a commonly used measure is the *mean squared error*.

Definition (Mean squared error)**.** The *mean squared error* of an estimator $\hat{\theta}$ is $\mathbb{E}_\theta[(\hat{\theta} - \theta)^2]$.

Sometimes, we use the *root mean squared error*, that is the square root of the above.

We can express the mean squared error in terms of the variance and bias:

$$\begin{aligned}\mathbb{E}_\theta[(\hat{\theta} - \theta)^2] &= \mathbb{E}_\theta[(\hat{\theta} - E_\theta(\hat{\theta}) + \mathbb{E}_\theta(\hat{\theta}) - \theta)^2] \\ &= \mathbb{E}_\theta[(\hat{\theta} - E_\theta(\hat{\theta}))^2] + [\mathbb{E}_\theta(\hat{\theta}) - \theta]^2 + 2[\mathbb{E}_\theta(\hat{\theta}) - \theta]\mathbb{E}_\theta[\hat{\theta} - \mathbb{E}_\theta(\hat{\theta})] \\ &= \mathrm{var}(\hat{\theta}) + \mathrm{bias}^2(\hat{\theta}).\end{aligned}$$

If we are aiming for a low mean squared error, sometimes it could be preferable to have a biased estimator with a lower variance. This is known as the "bias-variance trade-off".

For example, suppose $X \sim \text{binomial}(n, \theta)$. The standard estimator is $T_U = X/n$, which is unbiased. T_U has variance

$$\mathrm{var}_\theta(T_U) = \frac{\mathrm{var}_\theta(X)}{n^2} = \frac{\theta(1-\theta)}{n}.$$

Hence the mean squared error of the usual estimator is given by

$$\mathrm{mse}(T_U) = \mathrm{var}_\theta(T_U) + \mathrm{bias}^2(T_U) = \theta(1-\theta)/n.$$

Consider an alternative estimator

$$T_B = \frac{X+1}{n+2} = w\frac{X}{n} + (1-w)\frac{1}{2},$$

where $w = n/(n+2)$. This can be interpreted to be a weighted average (by the sample size) of the sample mean and $1/2$. We have

$$\mathbb{E}_\theta(T_B) - \theta = \frac{n\theta + 1}{n+2} - \theta = (1-w)\left(\frac{1}{2} - \theta\right),$$

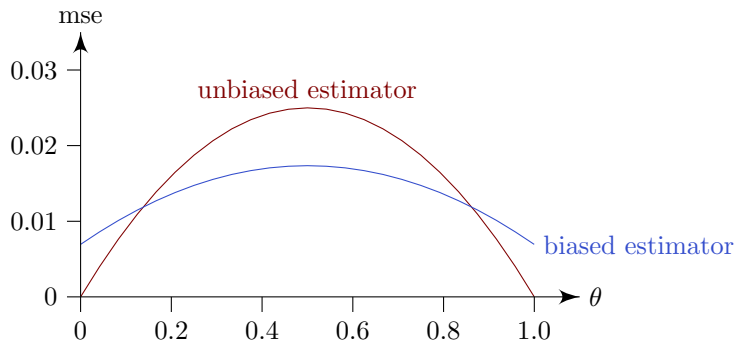
and is biased. The variance is given by

$$\mathrm{var}_\theta(T_B) = \frac{\mathrm{var}_\theta(X)}{(n+2)^2} = w^2\frac{\theta(1-\theta)}{n}.$$

Hence the mean squared error is

$$\text{mse}(T_B) = \text{var}_\theta(T_B) + \text{bias}^2(T_B) = w^2\frac{\theta(1-\theta)}{n} + (1-w)^2\left(\frac{1}{2} - \theta\right)^2.$$

We can plot the mean squared error of each estimator for possible values of θ. Here we plot the case where $n = 10$.



This biased estimator has smaller MSE unless θ has extreme values.

We see that sometimes biased estimators could give better mean squared errors. In some cases, not only could unbiased estimators be worse — they could be completely nonsense.

Suppose $X \sim \text{Poisson}(\lambda)$, and for some reason, we want to estimate $\theta = [P(X = 0)]^2 = e^{-2\lambda}$. Then any unbiased estimator $T(X)$ must satisfy $\mathbb{E}_\theta(T(X)) = \theta$, or equivalently,

$$E_\lambda(T(X)) = e^{-\lambda}\sum_{x=0}^{\infty} T(x)\frac{\lambda^x}{x!} = e^{-2\lambda}.$$

The only function T that can satisfy this equation is $T(X) = (-1)^X$.

Thus the unbiased estimator would estimate $e^{-2\lambda}$ to be 1 if X is even, -1 if X is odd. This is clearly nonsense.

1.3 Sufficiency

Often, we do experiments just to find out the value of θ. For example, we might want to estimate what proportion of the population supports some political candidate. We are seldom interested in the data points themselves, and just want to learn about the big picture. This leads us to the concept of a *sufficient statistic*. This is a statistic $T(\mathbf{X})$ that contains all information we have about θ in the sample.

Example. Let $X_1, \cdots X_n$ be iid Bernoulli(θ), so that $\mathbb{P}(X_i = 1) = 1 - \mathbb{P}(X_i = 0) = \theta$ for some $0 < \theta < 1$. So

$$f_{\mathbf{X}}(\mathbf{x} \mid \theta) = \prod_{i=1}^{n} \theta^{x_i}(1-\theta)^{1-x_i} = \theta^{\sum x_i}(1-\theta)^{n-\sum x_i}.$$

This depends on the data only through $T(\mathbf{X}) = \sum x_i$, the total number of ones.

Suppose we are now given that $T(\mathbf{X}) = t$. Then what is the distribution of $\mathbf{X}$? We have

$$f_{\mathbf{X}|T=t}(\mathbf{x}) = \frac{\mathbb{P}_\theta(\mathbf{X} = \mathbf{x}, T = t)}{\mathbb{P}_\theta(T = t)} = \frac{\mathbb{P}_\theta(\mathbf{X} = \mathbf{x})}{\mathbb{P}_\theta(T = t)}.$$

Where the last equality comes because since if $\mathbf{X} = \mathbf{x}$, then T must be equal to t. This is equal to

$$\frac{\theta^{\sum x_i}(1-\theta)^{n-\sum x_i}}{\binom{n}{t}\theta^t(1-\theta)^{n-t}} = \binom{n}{t}^{-1}.$$

So the conditional distribution of $\mathbf{X}$ given $T = t$ does not depend on θ. So if we know T, then additional knowledge of $\mathbf{x}$ does not give more information about θ.

Definition (Sufficient statistic)**.** A statistic T is *sufficient* for θ if the conditional distribution of $\mathbf{X}$ given T does not depend on θ.

There is a convenient theorem that allows us to find sufficient statistics.

Theorem (The factorization criterion)**.** T is sufficient for θ if and only if

$$f_{\mathbf{X}}(\mathbf{x} \mid \theta) = g(T(\mathbf{x}), \theta)h(\mathbf{x})$$

for some functions g and h.

Proof. We first prove the discrete case.

Suppose $f_{\mathbf{X}}(\mathbf{x} \mid \theta) = g(T(\mathbf{x}), \theta)h(\mathbf{x})$. If $T(\mathbf{x}) = t$, then

$$\begin{aligned} f_{\mathbf{X}|T=t}(\mathbf{x}) &= \frac{\mathbb{P}_\theta(\mathbf{X} = \mathbf{x}, T(\mathbf{X}) = t)}{\mathbb{P}_\theta(T = t)} \\ &= \frac{g(T(\mathbf{x}), \theta)h(\mathbf{x})}{\sum_{\{\mathbf{y}:T(\mathbf{y})=t\}} g(T(\mathbf{y}), \theta)h(\mathbf{y})} \\ &= \frac{g(t, \theta)h(\mathbf{x})}{g(t, \theta)\sum h(\mathbf{y})} \\ &= \frac{h(\mathbf{x})}{\sum h(\mathbf{y})} \end{aligned}$$

which doesn't depend on θ. So T is sufficient.

The continuous case is similar. If $f_{\mathbf{X}}(\mathbf{x} \mid \theta) = g(T(\mathbf{x}), \theta)h(\mathbf{x})$, and $T(\mathbf{x}) = t$, then

$$\begin{aligned} f_{\mathbf{X}|T=t}(\mathbf{x}) &= \frac{g(T(\mathbf{x}), \theta)h(\mathbf{x})}{\int_{\mathbf{y}:T(\mathbf{y})=t} g(T(\mathbf{y}), \theta)h(\mathbf{y})\, \mathrm{d}\mathbf{y}} \\ &= \frac{g(t, \theta)h(\mathbf{x})}{g(t, \theta)\int h(\mathbf{y})\, \mathrm{d}\mathbf{y}} \\ &= \frac{h(\mathbf{x})}{\int h(\mathbf{y})\, \mathrm{d}\mathbf{y}}, \end{aligned}$$

which does not depend on θ.

Now suppose T is sufficient so that the conditional distribution of $\mathbf{X} \mid T = t$ does not depend on θ. Then

$$\mathbb{P}_\theta(\mathbf{X} = \mathbf{x}) = \mathbb{P}_\theta(\mathbf{X} = \mathbf{x}, T = T(\mathbf{x})) = \mathbb{P}_\theta(\mathbf{X} = \mathbf{x} \mid T = T(\mathbf{x}))\mathbb{P}_\theta(T = T(\mathbf{x})).$$

The first factor does not depend on θ by assumption; call it $h(\mathbf{x})$. Let the second factor be $g(t, \theta)$, and so we have the required factorisation. □

Example. Continuing the above example,

$$f_{\mathbf{X}}(\mathbf{x} \mid \theta) = \theta^{\sum x_i}(1-\theta)^{n-\sum x_i}.$$

Take $g(t, \theta) = \theta^t(1-\theta)^{n-t}$ and $h(\mathbf{x}) = 1$ to see that $T(\mathbf{X}) = \sum X_i$ is sufficient for θ.

Example. Let $X_1, \cdots, X_n$ be iid $U[0, \theta]$. Write $1_{[A]}$ for the indicator function of an arbitrary set A. We have

$$f_{\mathbf{X}}(\mathbf{x} \mid \theta) = \prod_{i=1}^{n} \frac{1}{\theta} 1_{[0 \le x_i \le \theta]} = \frac{1}{\theta^n} 1_{[\max_i x_i \le \theta]} 1_{[\min_i x_i \ge 0]}.$$

If we let $T = \max_i x_i$, then we have

$$f_{\mathbf{X}}(\mathbf{x} \mid \theta) = \underbrace{\frac{1}{\theta^n} 1_{[t \le \theta]}}_{g(t,\theta)} \quad \underbrace{1_{[\min_i x_i \ge 0]}}_{h(\mathbf{x})}.$$

So $T = \max_i x_i$ is sufficient.

Note that sufficient statistics are not unique. If T is sufficient for θ, then so is any 1-1 function of T. $\mathbf{X}$ is always sufficient for θ as well, but it is not of much use. How can we decide if a sufficient statistic is "good"?

Given any statistic T, we can partition the sample space $\mathcal{X}^n$ into sets $\{\mathbf{x} \in \mathcal{X} : T(\mathbf{X}) = t\}$. Then after an experiment, instead of recording the actual value of $\mathbf{x}$, we can simply record the partition $\mathbf{x}$ falls into. If there are less partitions than possible values of $\mathbf{x}$, then effectively there is less information we have to store.

If T is sufficient, then this data reduction does not lose any information about θ. The "best" sufficient statistic would be one in which we achieve the maximum possible reduction. This is known as the *minimal sufficient statistic*. The formal definition we take is the following:

Definition (Minimal sufficiency)**.** A sufficient statistic $T(\mathbf{X})$ is *minimal* if it is a function of every other sufficient statistic, i.e. if $T'(\mathbf{X})$ is also sufficient, then $T'(\mathbf{X}) = T'(\mathbf{Y}) \Rightarrow T(\mathbf{X}) = T(\mathbf{Y})$.

Again, we have a handy theorem to find minimal statistics:

Theorem. Suppose $T = T(\mathbf{X})$ is a statistic that satisfies

$$\frac{f_{\mathbf{X}}(\mathbf{x}; \theta)}{f_{\mathbf{X}}(\mathbf{y}; \theta)} \text{ does not depend on } \theta \text{ if and only if } T(\mathbf{x}) = T(\mathbf{y}).$$

Then T is minimal sufficient for θ.

Proof. First we have to show sufficiency. We will use the factorization criterion to do so.

Firstly, for each possible t, pick a favorite $\mathbf{x}_t$ such that $T(\mathbf{x}_t) = t$.

Now let $\mathbf{x} \in \mathcal{X}^N$ and let $T(\mathbf{x}) = t$. So $T(\mathbf{x}) = T(\mathbf{x}_t)$. By the hypothesis, $\frac{f_{\mathbf{X}}(\mathbf{x};\theta)}{f_{\mathbf{X}}(\mathbf{x}_t;\theta)}$ does not depend on θ. Let this be $h(\mathbf{x})$. Let $g(t, \theta) = f_{\mathbf{X}}(\mathbf{x}_t, \theta)$. Then

$$f_{\mathbf{X}}(\mathbf{x}; \theta) = f_{\mathbf{X}}(\mathbf{x}_t; \theta) \frac{f_{\mathbf{X}}(\mathbf{x}; \theta)}{f_{\mathbf{X}}(\mathbf{x}_t; \theta)} = g(t, \theta) h(\mathbf{x}).$$

So T is sufficient for θ.

To show that this is minimal, suppose that $S(\mathbf{X})$ is also sufficient. By the factorization criterion, there exist functions g_S and h_S such that

$$f_{\mathbf{X}}(\mathbf{x};\theta) = g_S(S(\mathbf{x}),\theta)h_S(\mathbf{x}).$$

Now suppose that $S(\mathbf{x}) = S(\mathbf{y})$. Then

$$\frac{f_{\mathbf{X}}(\mathbf{x};\theta)}{f_{\mathbf{X}}(\mathbf{y};\theta)} = \frac{g_S(S(\mathbf{x}),\theta)h_S(\mathbf{x})}{g_S(S(\mathbf{y}),\theta)h_S(\mathbf{y})} = \frac{h_S(\mathbf{x})}{h_S(\mathbf{y})}.$$

This means that the ratio $\frac{f_{\mathbf{X}}(\mathbf{x};\theta)}{f_{\mathbf{X}}(\mathbf{y};\theta)}$ does not depend on θ. By the hypothesis, this implies that $T(\mathbf{x}) = T(\mathbf{y})$. So we know that $S(\mathbf{x}) = S(\mathbf{y})$ implies $T(\mathbf{x}) = T(\mathbf{y})$. So T is a function of S. So T is minimal sufficient. □

Example. Suppose $X_1, \cdots, X_n$ are iid $N(\mu, \sigma^2)$. Then

$$\begin{aligned}\frac{f_{\mathbf{X}}(\mathbf{x} \mid \mu,\sigma^2)}{f_{\mathbf{X}}(\mathbf{y} \mid \mu,\sigma^2)} &= \frac{(2\pi\sigma^2)^{-n/2}\exp\left\{-\frac{1}{2\sigma^2}\sum_i (x_i-\mu)^2\right\}}{(2\pi\sigma^2)^{-n/2}\exp\left\{-\frac{1}{2\sigma^2}\sum_i (y_i-\mu)^2\right\}}\\ &= \exp\left\{-\frac{1}{2\sigma^2}\left(\sum_i x_i^2 - \sum_i y_i^2\right) + \frac{\mu}{\sigma^2}\left(\sum_i x_i - \sum_i y_i\right)\right\}.\end{aligned}$$

This is a constant function of (μ, σ^2) iff $\sum_i x_i^2 = \sum_i y_i^2$ and $\sum_i x_i = \sum_i y_i$. So $T(\mathbf{X}) = (\sum_i X_i^2, \sum_i X_i)$ is minimal sufficient for (μ, σ^2).

As mentioned, minimal sufficient statistics allow us to store the results of our experiments in the most efficient way. It turns out if we have a minimal sufficient statistic, then we can use it to improve *any* estimator.

Theorem (Rao-Blackwell Theorem)**.** Let T be a sufficient statistic for θ and let $\tilde{\theta}$ be an estimator for θ with $\mathbb{E}(\tilde{\theta}^2) < \infty$ for all θ. Let $\hat{\theta}(\mathbf{x}) = \mathbb{E}[\tilde{\theta}(\mathbf{X}) \mid T(\mathbf{X}) = T(\mathbf{x})]$. Then for all θ,

$$\mathbb{E}[(\hat{\theta} - \theta)^2] \leq \mathbb{E}[(\tilde{\theta} - \theta)^2].$$

The inequality is strict unless $\tilde{\theta}$ is a function of T.

Here we have to be careful with our definition of $\hat{\theta}$. It is defined as the expected value of $\tilde{\theta}(\mathbf{X})$. And this could potentially depend on the actual value of θ. Fortunately, since T is sufficient for θ, the conditional distribution of $\mathbf{X}$ given $T = t$ does not depend on θ. Hence $\hat{\theta} = \mathbb{E}[\tilde{\theta}(\mathbf{X}) \mid T]$ does not depend on θ, and so is a genuine estimator.

Using this theorem, given any estimator, we can find one that is a function of a sufficient statistic and is at least as good in terms of mean squared error of estimation. Moreover, if the original estimator $\tilde{\theta}$ is unbiased, so is the new $\hat{\theta}$. Also, if $\tilde{\theta}$ is already a function of T, then $\hat{\theta} = \tilde{\theta}$.

Proof. By the conditional expectation formula, we have $\mathbb{E}(\hat{\theta}) = \mathbb{E}[\mathbb{E}(\tilde{\theta} \mid T)] = E(\tilde{\theta})$. So they have the same bias.

By the conditional variance formula,

$$\mathrm{var}(\tilde{\theta}) = \mathbb{E}[\mathrm{var}(\tilde{\theta} \mid T)] + \mathrm{var}[\mathbb{E}(\tilde{\theta} \mid T)] = \mathbb{E}[\mathrm{var}(\tilde{\theta} \mid T)] + \mathrm{var}(\hat{\theta}).$$

Hence $\mathrm{var}(\tilde{\theta}) \geq \mathrm{var}(\hat{\theta})$. So $\mathrm{mse}(\tilde{\theta}) \geq \mathrm{mse}(\hat{\theta})$, with equality only if $\mathrm{var}(\tilde{\theta} \mid T) = 0$. □

Example. Suppose $X_1, \cdots, X_n$ are iid Poisson(λ), and let $\theta = e^{-\lambda}$, which is the probability that $X_1 = 0$. Then

$$p_{\mathbf{X}}(\mathbf{x} \mid \lambda) = \frac{-e^{n\lambda}\lambda^{\sum x_i}}{\prod x_i!}.$$

So

$$p_{\mathbf{X}}(\mathbf{x} \mid \theta) = \frac{\theta^n(-\log\theta)^{\sum x_i}}{\prod x_i!}.$$

We see that $T = \sum X_i$ is sufficient for θ, and $\sum X_i \sim \text{Poisson}(n\lambda)$.

We start with an easy estimator θ is $\tilde{\theta} = 1_{X_1=0}$, which is unbiased (i.e. if we observe nothing in the first observation period, we assume the event is impossible). Then

$$\begin{aligned}\mathbb{E}[\tilde{\theta} \mid T = t] &= \mathbb{P}\left(X_1 = 0 \mid \sum_1^n X_i = t\right)\\ &= \frac{\mathbb{P}(X_1 = 0)\mathbb{P}(\sum_2^n X_i = t)}{\mathbb{P}(\sum_1^n X_i = t)}\\ &= \left(\frac{n-1}{n}\right)^t.\end{aligned}$$

So $\hat{\theta} = (1 - 1/n)^{\sum x_i}$. This approximately $(1 - 1/n)^{n\bar{X}} \approx e^{-\bar{X}} = e^{-\hat{\lambda}}$, which makes sense.

Example. Let $X_1, \cdots, X_n$ be iid $U[0, \theta]$, and suppose that we want to estimate θ. We have shown above that $T = \max X_i$ is sufficient for θ. Let $\hat{\theta} = 2X_1$, an unbiased estimator. Then

$$\begin{aligned}\mathbb{E}[\tilde{\theta} \mid T = t] &= 2\mathbb{E}[X_1 \mid \max X_i = t]\\ &= 2\mathbb{E}[X_1 \mid \max X_i = t, X_1 = \max X_i]\mathbb{P}(X_1 = \max X_i)\\ &\quad + 2\mathbb{E}[X_1 \mid \max X_i = t, X_1 \neq \max X_i]\mathbb{P}(X_1 \neq \max X_i)\\ &= 2\left(t \times \frac{1}{n} + \frac{t}{2}\frac{n-1}{n}\right)\\ &= \frac{n+1}{n}t.\end{aligned}$$

So $\hat{\theta} = \frac{n+1}{n}\max X_i$ is our new estimator.

1.4 Likelihood

There are many different estimators we can pick, and we have just come up with some criteria to determine whether an estimator is "good". However, these do not give us a systematic way of coming up with an estimator to actually use. In practice, we often use the *maximum likelihood estimator*.

Let $X_1, \cdots, X_n$ be random variables with joint pdf/pmg $f_{\mathbf{X}}(\mathbf{x} \mid \theta)$. We observe $\mathbf{X} = \mathbf{x}$.

Definition (Likelihood)**.** For any given $\mathbf{x}$, the *likelihood* of θ is $\text{like}(\theta) = f_{\mathbf{X}}(\mathbf{x} \mid \theta)$, regarded as a function of θ. The *maximum likelihood estimator* (mle) of θ is an estimator that picks the value of θ that maximizes $\text{like}(\theta)$.

Often there is no closed form for the mle, and we have to find $\hat{\theta}$ numerically.

When we can find the mle explicitly, in practice, we often maximize the *log-likelihood* instead of the likelihood. In particular, if $X_1, \cdots, X_n$ are iid, each with pdf/pmf $f_X(x \mid \theta)$, then

$$\text{like}(\theta) = \prod_{i=1}^{n} f_X(x_i \mid \theta),$$
$$\log \text{like}(\theta) = \sum_{i=1}^{n} \log f_X(x_i \mid \theta).$$

Example. Let $X_1, \cdots, X_n$ be iid Bernoulli(p). Then

$$l(p) = \log \text{like}(p) = \left(\sum x_i\right) \log p + \left(n - \sum x_i\right) \log(1-p).$$

Thus

$$\frac{\mathrm{d}l}{\mathrm{d}p} = \frac{\sum x_i}{p} - \frac{n - \sum x_i}{1-p}.$$

This is zero when $p = \sum x_i / n$. So this is the maximum likelihood estimator (and is unbiased).

Example. Let $X_1, \cdots, X_n$ be iid $N(\mu, \sigma^2)$, and we want to estimate $\theta = (\mu, \sigma^2)$. Then

$$l(\mu, \sigma^2) = \log \text{like}(\mu, \sigma^2) = -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} \sum (x_i - \mu)^2.$$

This is maximized when

$$\frac{\partial l}{\partial \mu} = \frac{\partial l}{\partial \sigma^2} = 0.$$

We have

$$\frac{\partial l}{\partial \mu} = -\frac{1}{\sigma^2} \sum (x_i - \mu), \quad \frac{\partial l}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \sum (x_i - \mu)^2.$$

So the solution, hence maximum likelihood estimator is $(\hat{\mu}, \hat{\sigma}^2) = (\bar{x}, S_{xx}/n)$, where $\bar{x} = \frac{1}{n} \sum x_i$ and $S_{xx} = \sum (x_i - \bar{x})^2$.

We shall see later that $S_{XX}/\sigma^2 = \frac{n\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-1}$, and so $\mathbb{E}(\hat{\sigma}^2) = \frac{(n-1)\sigma^2}{n}$, i.e. $\hat{\sigma}^2$ is biased.

Example (German tank problem)**.** Suppose the American army discovers some German tanks that are sequentially numbered, i.e. the first tank is numbered 1, the second is numbered 2, etc. Then if θ tanks are produced, then the probability distribution of the tank number is $U(0, \theta)$. Suppose we have discovered n tanks whose numbers are $x_1, x_2, \cdots, x_n$, and we want to estimate θ, the total number of tanks produced. We want to find the maximum likelihood estimator.

Then

$$\text{like}(\theta) = \frac{1}{\theta^n} 1_{[\max x_i \le \theta]} 1_{[\min x_i \ge 0]}.$$

So for $\theta \ge \max_i$, $\text{like}(\theta) = 1/\theta^n$ and is decreasing as θ increases, while for $\theta < \max x_i$, $\text{like}(\theta) = 0$. Hence the value $\hat{\theta} = \max x_i$ maximizes the likelihood.

Is $\hat{\theta}$ unbiased? First we need to find the distribution of $\hat{\theta}$. For $0 \le t \le \theta$, the cumulative distribution function of $\hat{\theta}$ is

$$F_{\hat{\theta}}(t) = P(\hat{\theta} \le t) = \mathbb{P}(X_i \le t \text{ for all } i) = (\mathbb{P}(X_i \le t))^n = \left(\frac{t}{\theta}\right)^n,$$

Differentiating with respect to T, we find the pdf $f_{\hat{\theta}} = \frac{nt^{n-1}}{\theta^n}$. Hence

$$\mathbb{E}(\hat{\theta}) = \int_0^\theta t\frac{nt^{n-1}}{\theta^n}\,\mathrm{d}t = \frac{n\theta}{n+1}.$$

So $\hat{\theta}$ is biased, but asymptotically unbiased.

Example. Smarties come in k equally frequent colours, but suppose we do not know k. Assume that we sample with replacement (although this is unhygienic).

Our first Smarties are Red, Purple, Red, Yellow. Then

$$\begin{aligned}\text{like}(k) &= \mathbb{P}_k(\text{1st is a new colour})\mathbb{P}_k(\text{2nd is a new colour})\\ &\qquad \mathbb{P}_k(\text{3rd matches 1st})\mathbb{P}_k(\text{4th is a new colour})\\ &= 1 \times \frac{k-1}{k} \times \frac{1}{k} \times \frac{k-2}{k}\\ &= \frac{(k-1)(k-2)}{k^3}.\end{aligned}$$

The maximum likelihood is 5 (by trial and error), even though it is not much likelier than the others.

How does the mle relate to sufficient statistics? Suppose that T is sufficient for θ. Then the likelihood is $g(T(\mathbf{x}), \theta)h(\mathbf{x})$, which depends on θ through $T(\mathbf{x})$. To maximise this as a function of θ, we only need to maximize g. So the mle $\hat{\theta}$ is a function of the sufficient statistic.

Note that if $\phi = h(\theta)$ with h injective, then the mle of ϕ is given by $h(\hat{\theta})$. For example, if the mle of the standard deviation σ is $\hat{\sigma}$, then the mle of the variance σ^2 is $\hat{\sigma}^2$. This is rather useful in practice, since we can use this to simplify a lot of computations.

1.5 Confidence intervals

Definition. A $100\gamma\%$ $(0 < \gamma < 1)$ *confidence interval* for θ is a random interval $(A(\mathbf{X}), B(\mathbf{X}))$ such that $\mathbb{P}(A(\mathbf{X}) < \theta < B(\mathbf{X})) = \gamma$, no matter what the true value of θ may be.

It is also possible to have confidence intervals for vector parameters.

Notice that it is the endpoints of the interval that are random quantities, while θ is a fixed constant we want to find out.

We can interpret this in terms of repeat sampling. If we calculate $(A(\mathbf{x}), B(\mathbf{x}))$ for a large number of samples $\mathbf{x}$, then approximately $100\gamma\%$ of them will cover the true value of θ.

It is important to know that having observed some data $\mathbf{x}$ and calculated 95% confidence interval, we *cannot* say that θ has 95% chance of being within the interval. Apart from the standard objection that θ is a fixed value and either is or is not in the interval, and hence we cannot assign probabilities to this event, we will later construct an example where even though we have got a 50% confidence interval, we are 100% sure that θ lies in that interval.

Example. Suppose $X_1, \cdots, X_n$ are iid $N(\theta, 1)$. Find a 95% confidence interval for θ.

We know $\bar{X} \sim N(\theta, \frac{1}{n})$, so that $\sqrt{n}(\bar{X} - \theta) \sim N(0, 1)$.

Let z_1, z_2 be such that $\phi(z_2) - \phi(z_1) = 0.95$, where ϕ is the standard normal distribution function.

We have $\mathbb{P}[z_1 < \sqrt{n}(\bar{X} - \theta) < z_2] = 0.95$, which can be rearranged to give

$$\mathbb{P}\left[\bar{X} - \frac{z_2}{\sqrt{n}} < \theta < \bar{X} - \frac{z_1}{\sqrt{n}}\right] = 0.95.$$

so we obtain the following 95% confidence interval:

$$\left(\bar{X} - \frac{z_2}{\sqrt{n}}, \bar{X} - \frac{z_1}{\sqrt{n}}\right).$$

There are many possible choices for z_1 and z_2. Since $N(0, 1)$ density is symmetric, the shortest such interval is obtained by $z_2 = z_{0.025} = -z_1$. We can also choose other values such as $z_1 = -\infty$, $z_2 = 1.64$, but we usually choose symmetric end points.

The above example illustrates a common procedure for finding confidence intervals:

- Find a quantity $R(\mathbf{X}, \theta)$ such that the $\mathbb{P}_\theta$-distribution of $R(\mathbf{X}, \theta)$ does not depend on θ. This is called a *pivot*. In our example, $R(\mathbf{X}, \theta) = \sqrt{n}(\bar{X} - \theta)$.
- Write down a probability statement of the form $\mathbb{P}_\theta(c_1 < R(\mathbf{X}, \theta) < c_2) = \gamma$.
- Rearrange the inequalities inside $\mathbb{P}(\ldots)$ to find the interval.

Usually c_1, c_2 are percentage points from a known standardised distribution, often equitailed. For example, we pick 2.5% and 97.5% points for a 95% confidence interval. We could also use, say 0% and 95%, but this generally results in a wider interval.

Note that if $(A(\mathbf{x}), B(\mathbf{x}))$ is a $100\gamma\%$ confidence interval for θ, and $T(\theta)$ is a monotone increasing function of θ, then $(T(A(\mathbf{x})), T(B(\mathbf{x})))$ is a $100\gamma\%$ confidence interval for $T(\theta)$.

Example. Suppose $X_1, \cdots, X_{50}$ are iid $N(0, \sigma^2)$. Find a 99% confidence interval for σ^2.

We know that $X_i/\sigma \sim N(0, 1)$. So $\dfrac{1}{\sigma^2}\displaystyle\sum_{i=1}^{50} X_i^2 \sim \chi^2_{50}$.

So $R(\mathbf{X}, \sigma^2) = \sum_{i=1}^{50} X_2^2/\sigma^2$ is a pivot.

Recall that $\chi^2_n(\alpha)$ is the upper $100\alpha\%$ point of χ^2_n, i.e.

$$\mathbb{P}(\chi^2_n \leq \chi^2_n(\alpha)) = 1 - \alpha.$$

So we have $c_1 = \chi^2_{50}(0.995) = 27.99$ and $c_2 = \chi^2_{50}(0.005) = 79.49$.

So

$$\mathbb{P}\left(c_1 < \frac{\sum X_i^2}{\sigma^2} < c_2\right) = 0.99,$$

and hence

$$\mathbb{P}\left(\frac{\sum X_i^2}{c_2} < \sigma^2 < \frac{\sum X_i^2}{c_1}\right) = 0.99.$$

Using the remark above, we know that a 99% confidence interval for σ is $\left(\sqrt{\frac{\sum X_i^2}{c_2}}, \sqrt{\frac{\sum X_i^2}{c_1}}\right)$.

Example. Suppose $X_1, \cdots, X_n$ are iid Bernoulli(p). Find an approximate confidence interval for p.

The mle of p is $\hat{p} = \sum X_i/n$.

By the Central Limit theorem, $\hat{p}$ is approximately $N(p, p(1-p)/n)$ for large n.

So $\frac{\sqrt{n}(\hat{p}-p)}{\sqrt{p(1-p)}}$ is approximately $N(0,1)$ for large n. So we have

$$\mathbb{P}\left(\hat{p} - z_{(1-\gamma)/2}\sqrt{\frac{p(1-p)}{n}} < p < \hat{p} + z_{(1-\gamma)/2}\sqrt{\frac{p(1-p)}{n}}\right) \approx \gamma.$$

But p is unknown! So we approximate it by $\hat{p}$ to get a confidence interval for p when n is large:

$$\mathbb{P}\left(\hat{p} - z_{(1-\gamma)/2}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}} < p < \hat{p} + z_{(1-\gamma)/2}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}}\right) \approx \gamma.$$

Note that we have made a lot of approximations here, but it would be difficult to do better than this.

Example. Suppose an opinion poll says 20% of the people are going to vote UKIP, based on a random sample of $1,000$ people. What might the true proportion be?

We assume we have an observation of $x = 200$ from a binomial(n, p) distribution with $n = 1,000$. Then $\hat{p} = x/n = 0.2$ is an unbiased estimate, and also the mle.

Now $\text{var}(X/n) = \frac{p(1-p)}{n} \approx \frac{\hat{p}(1-\hat{p})}{n} = 0.00016$. So a 95% confidence interval is

$$\left(\hat{p} - 1.96\sqrt{\frac{\hat{p}(1-\hat{p})}{n}}, \hat{p} + 1.96\sqrt{\frac{\hat{p}(1-\hat{p})}{n}}\right) = 0.20 \pm 1.96 \times 0.013 = (0.175, 0.225),$$

If we don't want to make that many approximations, we can note that $p(1-p) \leq 1/4$ for all $0 \leq p \leq 1$. So a conservative 95% interval is $\hat{p} \pm 1.96\sqrt{1/4n} \approx \hat{p} \pm \sqrt{1/n}$. So whatever proportion is reported, it will be 'accurate' to $\pm 1/\sqrt{n}$.

Example. Suppose X_1, X_2 are iid from $U(\theta - 1/2, \theta + 1/2)$. What is a sensible 50% confidence interval for θ?

We know that each X_i is equally likely to be less than θ or greater than θ. So there is 50% chance that we get one observation on each side, i.e.

$$\mathbb{P}_\theta(\min(X_1, X_2) \leq \theta \leq \max(X_1, X_2)) = \frac{1}{2}.$$

So $(\min(X_1, X_2), \max(X_1, X_2))$ is a 50% confidence interval for θ.

But suppose after the experiment, we obtain $|x_1 - x_2| \geq \frac{1}{2}$. For example, we might get $x_1 = 0.2, x_2 = 0.9$, then we *know* that, in this particular case, θ *must* lie in $(\min(X_1, X_2), \max(X_1, X_2))$, and we don't have just 50% "confidence"!

This is why after we calculate a confidence interval, we should not say "there is $100(1-\alpha)\%$ chance that θ lies in here". The confidence interval just says that "if we keep making these intervals, $100(1-\alpha)\%$ of them will contain θ". But if have calculated a *particular* confidence interval, the probability that that *particular* interval contains θ is *not* $100(1-\alpha)\%$.

1.6 Bayesian estimation

So far we have seen the *frequentist* approach to a statistical inference, i.e. inferential statements about θ are interpreted in terms of repeat sampling. For example, the confidence interval is what's the probability that the interval will contain θ, not the probability that θ lies in the interval.

In contrast, the Bayesian approach treats θ as a random variable taking values in Θ. The investigator's information and beliefs about the possible values of θ before any observation of data are summarised by a *prior distribution* $\pi(\theta)$. When $\mathbf{X} = \mathbf{x}$ are observed, the extra information about θ is combined with the prior to obtain the *posterior distribution* $\pi(\theta \mid \mathbf{x})$ for θ given $\mathbf{X} = \mathbf{x}$.

There has been a long-running argument between the two approaches. Recently, things have settled down, and Bayesian methods are seen to be appropriate in huge numbers of application where one seeks to assess a probability about a "state of the world". For example, spam filters will assess the probability that a specific email is a spam, even though from a frequentist's point of view, this is nonsense, because the email either is or is not a spam, and it makes no sense to assign a probability to the email's being a spam.

In Bayesian inference, we usually have some *prior* knowledge about the distribution of θ (e.g. between 0 and 1). After collecting some data, we will find a *posterior* distribution of θ given $\mathbf{X} = \mathbf{x}$.

Definition (Prior and posterior distribution)**.** The *prior distribution* of θ is the probability distribution of the value of θ before conducting the experiment. We usually write as $\pi(\theta)$.

The *posterior distribution* of θ is the probability distribution of the value of θ given an outcome of the experiment $\mathbf{x}$. We write as $\pi(\theta \mid \mathbf{x})$.

By Bayes' theorem, the distributions are related by

$$\pi(\theta \mid \mathbf{x}) = \frac{f_{\mathbf{X}}(\mathbf{x} \mid \theta)\pi(\theta)}{f_{\mathbf{X}}(\mathbf{x})}.$$

Thus

$$\pi(\theta \mid \mathbf{x}) \propto f_{\mathbf{X}}(\mathbf{x} \mid \theta)\pi(\theta).$$
$$\text{posterior} \propto \text{likelihood} \times \text{prior}.$$

where the constant of proportionality is chosen to make the total mass of the posterior distribution equal to one. Usually, we use this form, instead of attempting to calculate $f_{\mathbf{X}}(\mathbf{x})$.

It should be clear that the data enters through the likelihood, so the inference is automatically based on any sufficient statistic.

Example. Suppose I have 3 coins in my pocket. One is $3:1$ in favour of tails, one is a fair coin, and one is $3:1$ in favour of heads.

I randomly select one coin and flip it once, observing a head. What is the probability that I have chosen coin 3?

Let $X = 1$ denote the event that I observe a head, $X = 0$ if a tail. Let θ denote the probability of a head. So θ is either 0.25, 0.5 or 0.75.

Our prior distribution is $\theta(\theta = 0.25) = \pi(\theta = 0.5) = \pi(\theta = 0.75) = 1/3$.

The probability mass function $f_X(x \mid \theta) = \theta^x(1-\theta)^{1-x}$. So we have to following results:

θ	$\pi(\theta)$	$f_X(x=1 \mid \theta)$	$f_X(x=1 \mid \theta)\pi(\theta)$	$\pi(x)$
0.25	0.33	0.25	0.0825	0.167
0.50	0.33	0.50	0.1650	0.333
0.75	0.33	0.75	0.2475	0.500
Sum	1.00	1.50	0.4950	1.000

So if we observe a head, then there is now a 50% chance that we have picked the third coin.

Example. Suppose we are interested in the true mortality risk θ in a hospital H which is about to try a new operation. On average in the country, around 10% of the people die, but mortality rates in different hospitals vary from around 3% to around 20%. Hospital H has no deaths in their first 10 operations. What should we believe about θ?

Let $X_i = 1$ if the ith patient in H dies. The

$$f_{\mathbf{x}}(\mathbf{x} \mid \theta) = \theta^{\sum x_i}(1-\theta)^{n-\sum x_i}.$$

Suppose a priori that $\theta \sim \text{beta}(a, b)$ for some unknown $a > 0, b > 0$ so that

$$\pi(\theta) \propto \theta^{a-1}(1-\theta)^{b-1}.$$

Then the posteriori is

$$\pi(\theta \mid \mathbf{x}) \propto f_{\mathbf{x}}(\mathbf{x} \mid \theta)\pi(\theta) \propto \theta^{\sum x_i + a - 1}(1-\theta)^{n - \sum x_i + b - 1}.$$

We recognize this as $\text{beta}(\sum x_i + a, n - \sum x_i + b)$. So

$$\pi(\theta \mid \mathbf{x}) = \frac{\theta^{\sum x_i + a - 1}(1-\theta)^{n - \sum x_i + b - 1}}{B(\sum x_i + a, n - \sum x_i + b)}.$$

In practice, we need to find a Beta prior distribution that matches our information from other hospitals. It turns out that $\text{beta}(a = 3, b = 27)$ prior distribution has mean 0.1 and $\mathbb{P}(0.03 < \theta < .20) = 0.9$.

Then we observe data $\sum x_i = 0$, $n = 0$. So the posterior is $\text{beta}(\sum x_i + a, n - \sum x_i + b) = \text{beta}(3, 37)$. This has a mean of $3/40 = 0.075$.

This leads to a different conclusion than a frequentist analysis. Since nobody has died so far, the mle is 0, which does not seem plausible. Using a Bayesian approach, we have a higher mean than 0 because we take into account the data from other hospitals.

For this problem, a beta prior leads to a beta posterior. We say that the beta family is a *conjugate* family of prior distribution for Bernoulli samples.

Suppose that $a = b = 1$ so that $\pi(\theta) = 1$ for $0 < \theta < 1$ — the uniform distribution. Then the posterior is $\text{beta}(\sum x_i + 1, n - \sum x_i + 1)$, with properties

	mean	mode	variance
prior	$1/2$	non-unique	$1/12$
posterior	$\frac{\sum x_i + 1}{n+2}$	$\frac{\sum x_i}{n}$	$\frac{(\sum x_i + 1)(n - \sum x_i + 1)}{(n+2)^2(n+3)}$

Note that the mode of the posterior is the mle.

The posterior mean estimator, $\frac{\sum x_i+1}{n+2}$ is discussed in Lecture 2, where we showed that this estimator had smaller mse than the mle for non-extreme value of θ. This is known as the Laplace's estimator.

The posterior variance is bounded above by $1/(4(n+3))$, and this is smaller than the prior variance, and is smaller for larger n.

Again, note that the posterior automatically depends on the data through the sufficient statistic.

After we come up with the posterior distribution, we have to decide what estimator to use. In the case above, we used the posterior mean, but this might not be the best estimator.

To determine what is the "best" estimator, we first need a *loss function*. Let $L(\theta, a)$ be the loss incurred in estimating the value of a parameter to be a when the true value is θ.

Common loss functions are quadratic loss $L(\theta, a) = (\theta - a)^2$, absolute error loss $L(\theta, a) = |\theta - a|$, but we can have others.

When our estimate is a, the expected posterior loss is

$$h(a) = \int L(\theta, a)\pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta.$$

Definition (Bayes estimator)**.** The *Bayes estimator* $\hat{\theta}$ is the estimator that minimises the expected posterior loss.

For quadratic loss,

$$h(a) = \int (a - \theta)^2 \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta.$$

$h'(a) = 0$ if

$$\int (a - \theta)\pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta = 0,$$

or

$$a \int \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta = \int \theta \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta,$$

Since $\int \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta = 1$, the Bayes estimator is $\hat{\theta} = \int \theta \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta$, the *posterior mean*.

For absolute error loss,

$$\begin{aligned} h(a) &= \int |\theta - a| \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta \\ &= \int_{-\infty}^{a} (a - \theta)\pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta + \int_{a}^{\infty} (\theta - a)\pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta \\ &= a \int_{-\infty}^{a} \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta - \int_{-\infty}^{a} \theta \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta \\ &+ \int_{a}^{\infty} \theta \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta - a \int_{a}^{\infty} \pi(\theta \mid \mathbf{x}) \, \mathrm{d}\theta. \end{aligned}$$

Now $h'(a) = 0$ if

$$\int_{-\infty}^{a} \pi(\theta \mid \mathbf{x})\, \mathrm{d}\theta = \int_{a}^{\infty} \pi(\theta \mid \mathbf{x})\, \mathrm{d}\theta.$$

This occurs when each side is $1/2$. So $\hat{\theta}$ is the *posterior median*.

Example. Suppose that $X_1, \cdots, X_n$ are iid $N(\mu, 1)$, and that a prior $\mu \sim N(0, \tau^{-2})$ for some τ^{-2}. So τ is the certainty of our prior knowledge.

The posterior is given by

$$\begin{aligned}\pi(\mu \mid \mathbf{x}) &\propto f_{\mathbf{x}}(\mathbf{x} \mid \mu)\pi(\mu)\\ &\propto \exp\left[-\frac{1}{2}\sum (x_i - \mu)^2\right] \exp\left[-\frac{\mu^2\tau^2}{2}\right]\\ &\propto \exp\left[-\frac{1}{2}(n+\tau^2)\left\{\mu - \frac{\sum x_i}{n+\tau^2}\right\}^2\right]\end{aligned}$$

which is a normal distribution. So the posterior distribution of μ given $\mathbf{x}$ is a normal distribution with mean $\sum x_i/(n+\tau^2)$ and variance $1/(n+\tau^2)$.

The normal density is symmetric, and so the posterior mean and the posterior media have the same value $\sum x_i/(n+\tau^2)$.

This is the optimal estimator for both quadratic and absolute loss.

Example. Suppose that $X_1, \cdots, X_n$ are iid Poisson(λ) random variables, and λ has an exponential distribution with mean 1. So $\pi(\lambda) = e^{-\lambda}$.

The posterior distribution is given by

$$\pi(\lambda \mid \mathbf{x}) \propto e^{n\lambda}\lambda^{\sum x_i} e^{-\lambda} = \lambda^{\sum x_i} e^{-(n+1)\lambda}, \quad \lambda > 0,$$

which is gamma $(\sum x_i + 1, n+1)$. Hence under quadratic loss, our estimator is

$$\hat{\lambda} = \frac{\sum x_i + 1}{n+1},$$

the posterior mean.

Under absolute error loss, $\hat{\lambda}$ solves

$$\int_0^{\lambda} \frac{(n+1)^{\sum x_i + 1}\lambda^{\sum x_i} e^{-(n+1)\lambda}}{(\sum x_i)!}\, \mathrm{d}\lambda = \frac{1}{2}.$$

2 Hypothesis testing

Often in statistics, we have some *hypothesis* to test. For example, we want to test whether a drug can lower the chance of a heart attack. Often, we will have two hypotheses to compare: the *null hypothesis* states that the drug is useless, while the *alternative hypothesis* states that the drug is useful. Quantitatively, suppose that the chance of heart attack without the drug is θ_0 and the chance with the drug is θ. Then the null hypothesis is $H_0 : \theta = \theta_0$, while the alternative hypothesis is $H_1 : \theta \neq \theta_0$.

It is important to note that the null hypothesis and alternative hypothesis are not on equal footing. By default, we assume the null hypothesis is true. For us to reject the null hypothesis, we need a *lot* of evidence to prove that. This is since we consider incorrectly rejecting the null hypothesis to be a much more serious problem than accepting it when we should not. For example, it is relatively okay to reject a drug when it is actually useful, but it is terrible to distribute drugs to patients when the drugs are actually useless. Alternatively, it is more serious to deem an innocent person guilty than to say a guilty person is innocent.

In general, let $X_1, \cdots, X_n$ be iid, each taking values in $\mathcal{X}$, each with unknown pdf/pmf f. We have two hypotheses, H_0 and H_1, about f. On the basis of data $\mathbf{X} = \mathbf{x}$, we make a choice between the two hypotheses.

Example.

- A coin has $\mathbb{P}(\text{Heads}) = \theta$, and is thrown independently n times. We could have $H_0 : \theta = \frac{1}{2}$ versus $H_1 : \theta = \frac{3}{4}$.
- Suppose $X_1, \cdots, X_n$ are iid discrete random variables. We could have H_0 : the distribution is Poisson with unknown mean, and H_1 : the distribution is not Poisson.
- General parametric cases: Let $X_1, \cdots, X_n$ be iid with density $f(x \mid \theta)$. f is known while θ is unknown. Then our hypotheses are $H_0 : \theta \in \Theta_0$ and $H_1 : \theta \in \Theta_1$, with $\Theta_0 \cap \Theta_1 = \emptyset$.
- We could have $H_0 : f = f_0$ and $H_1 = f = f_1$, where f_0 and f_1 are densities that are completely specified but do not come form the same parametric family.

Definition (Simple and composite hypotheses)**.** A *simple hypothesis* H specifies f completely (e.g. $H_0 : \theta = \frac{1}{2}$). Otherwise, H is a *composite hypothesis*.

2.1 Simple hypotheses

Definition (Critical region)**.** For testing H_0 against an alternative hypothesis H_1, a test procedure has to partition $\mathcal{X}^n$ into two disjoint exhaustive regions C and $\bar{C}$, such that if $\mathbf{x} \in C$, then H_0 is rejected, and if $\mathbf{x} \in \bar{C}$, then H_0 is not rejected. C is the *critical region*.

When performing a test, we may either arrive at a correct conclusion, or make one of the two types of error:

Definition (Type I and II error)**.**

(i) *Type I error*: reject H_0 when H_0 is true.

(ii) *Type II error*: not rejecting H_0 when H_0 is false.

Definition (Size and power)**.** When H_0 and H_1 are both simple, let

$$\alpha = \mathbb{P}(\text{Type I error}) = \mathbb{P}(\mathbf{X} \in C \mid H_0 \text{ is true}).$$

$$\beta = \mathbb{P}(\text{Type II error}) = \mathbb{P}(\mathbf{X} \notin C \mid H_1 \text{ is true}).$$

The *size* of the test is α, and $1 - \beta$ is the *power* of the test to detect H_1.

If we have two simple hypotheses, a relatively straightforward test is the *likelihood ratio test*.

Definition (Likelihood)**.** The *likelihood* of a simple hypothesis $H : \theta = \theta^*$ given data $\mathbf{x}$ is

$$L_{\mathbf{x}}(H) = f_{\mathbf{X}}(\mathbf{x} \mid \theta = \theta^*).$$

The *likelihood ratio* of two simple hypotheses H_0, H_1 given data $\mathbf{x}$ is

$$\Lambda_{\mathbf{x}}(H_0; H_1) = \frac{L_{\mathbf{x}}(H_1)}{L_{\mathbf{x}}(H_0)}.$$

A *likelihood ratio test* (LR test) is one where the critical region C is of the form

$$C = \{\mathbf{x} : \Lambda_{\mathbf{x}}(H_0; H_1) > k\}$$

for some k.

It turns out this rather simple test is "the best" in the following sense:

Lemma (Neyman-Pearson lemma)**.** Suppose $H_0 : f = f_0$, $H_1 : f = f_1$, where f_0 and f_1 are continuous densities that are nonzero on the same regions. Then among all tests of size less than or equal to α, the test with the largest power is the likelihood ratio test of size α.

Proof. Under the likelihood ratio test, our critical region is

$$C = \left\{\mathbf{x} : \frac{f_1(\mathbf{x})}{f_0(\mathbf{x})} > k\right\},$$

where k is chosen such that $\alpha = \mathbb{P}(\text{reject } H_0 \mid H_0) = \mathbb{P}(\mathbf{X} \in C \mid H_0) = \int_C f_0(\mathbf{x})\, \mathrm{d}\mathbf{x}$. The probability of Type II error is given by

$$\beta = \mathbb{P}(\mathbf{X} \notin C \mid f_1) = \int_{\bar{C}} f_1(\mathbf{x})\, \mathrm{d}\mathbf{x}.$$

Let C^* be the critical region of any other test with size less than or equal to α. Let $\alpha^* = \mathbb{P}(X \in C^* \mid f_0)$ and $\beta^* = \mathbb{P}(\mathbf{X} \notin C^* \mid f_1)$. We want to show $\beta \leq \beta^*$.

We know $\alpha^* \leq \alpha$, ie

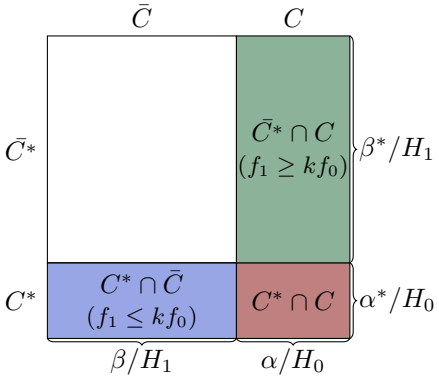
$$\int_{C^*} f_0(\mathbf{x})\, \mathrm{d}\mathbf{x} \leq \int_C f_0(\mathbf{x})\, \mathrm{d}\mathbf{x}.$$

Also, on C, we have $f_1(\mathbf{x}) > kf_0(\mathbf{x})$, while on $\bar{C}$ we have $f_1(\mathbf{x}) \leq kf_0(\mathbf{x})$. So

$$\int_{\bar{C}^* \cap C} f_1(\mathbf{x})\, d\mathbf{x} \geq k \int_{\bar{C}^* \cap C} f_0(\mathbf{x})\, d\mathbf{x}$$
$$\int_{\bar{C} \cap C^*} f_1(\mathbf{x})\, d\mathbf{x} \leq k \int_{\bar{C} \cap C^*} f_0(\mathbf{x})\, d\mathbf{x}.$$

Hence

$$\begin{aligned}
\beta - \beta^* &= \int_{\bar{C}} f_1(\mathbf{x})\, d\mathbf{x} - \int_{\bar{C}^*} f_1(\mathbf{x})\, d\mathbf{x} \\
&= \int_{\bar{C} \cap C^*} f_1(\mathbf{x})\, d\mathbf{x} + \int_{\bar{C} \cap \bar{C}^*} f_1(\mathbf{x})\, d\mathbf{x} \\
&\quad - \int_{\bar{C}^* \cap C} f_1(\mathbf{x})\, d\mathbf{x} - \int_{\bar{C} \cap \bar{C}^*} f_1(\mathbf{x})\, d\mathbf{x} \\
&= \int_{\bar{C} \cap C^*} f_1(\mathbf{x})\, d\mathbf{x} - \int_{\bar{C}^* \cap C} f_1(\mathbf{x})\, d\mathbf{x} \\
&\leq k \int_{\bar{C} \cap C^*} f_0(\mathbf{x})\, d\mathbf{x} - k \int_{\bar{C}^* \cap C} f_0(\mathbf{x})\, d\mathbf{x} \\
&= k \left\{ \int_{\bar{C} \cap C^*} f_0(\mathbf{x})\, d\mathbf{x} + \int_{C \cap C^*} f_0(\mathbf{x})\, d\mathbf{x} \right\} \\
&\quad - k \left\{ \int_{\bar{C}^* \cap C} f_0(\mathbf{x})\, d\mathbf{x} + \int_{C \cap C^*} f_0(\mathbf{x})\, d\mathbf{x} \right\} \\
&= k(\alpha^* - \alpha) \\
&\leq 0.
\end{aligned}$$



□

Here we assumed the f_0 and f_1 are continuous densities. However, this assumption is need just to ensure that the likelihood ratio test of exactly size α exists. Even with non-continuous distributions, the likelihood ratio test is still a good idea. In fact, you will show in the example sheets that for a discrete distribution, as long as a likelihood ratio test of exactly size α exists, the same result holds.

Example. Suppose $X_1, \cdots, X_n$ are iid $N(\mu, \sigma_0^2)$, where σ_0^2 is known. We want to find the best size α test of $H_0 : \mu = \mu_0$ against $H_1 : \mu = \mu_1$, where μ_0 and μ_1

are known fixed values with $\mu_1 > \mu_0$. Then

$$\Lambda_{\mathbf{x}}(H_0; H_1) = \frac{(2\pi\sigma_0^2)^{-n/2} \exp\left(-\frac{1}{2\sigma_0^2}\sum(x_i-\mu_1)^2\right)}{(2\pi\sigma_0^2)^{-n/2} \exp\left(-\frac{1}{2\sigma_0^2}\sum(x_i-\mu_0)^2\right)}$$
$$= \exp\left(\frac{\mu_1-\mu_0}{\sigma_0^2} n\bar{x} + \frac{n(\mu_0^2-\mu_1^2)}{2\sigma_0^2}\right).$$

This is an increasing function of $\bar{x}$, so for any k, $\Lambda_x > k \Leftrightarrow \bar{x} > c$ for some c. Hence we reject H_0 if $\bar{x} > c$, where c is chosen such that $\mathbb{P}(\bar{X} > c \mid H_0) = \alpha$.

Under H_0, $\bar{X} \sim N(\mu_0, \sigma_0^2/n)$, so $Z = \sqrt{n}(\bar{X}-\mu_0)/\sigma_0 \sim N(0,1)$.

Since $\bar{x} > c \Leftrightarrow z > c'$ for some c', the size α test rejects H_0 if

$$z = \frac{\sqrt{n}(\bar{x}-\mu_0)}{\sigma_0} > z_\alpha.$$

For example, suppose $\mu_0 = 5$, $\mu_1 = 6$, $\sigma_0 = 1$, $\alpha = 0.05$, $n = 4$ and $\mathbf{x} = (5.1, 5.5, 4.9, 5.3)$. So $\bar{x} = 5.2$.

From tables, $z_{0.05} = 1.645$. We have $z = 0.4$ and this is less than 1.645. So $\mathbf{x}$ is not in the rejection region.

We do not reject H_0 at the 5% level and say that the data are consistent with H_0.

Note that this does not mean that we *accept* H_0. While we don't have sufficient reason to believe it is false, we also don't have sufficient reason to believe it is true.

This is called a *z-test*.

In this example, LR tests reject H_0 if $z > k$ for some constant k. The size of such a test is $\alpha = \mathbb{P}(Z > k \mid H_0) = 1 - \Phi(k)$, and is decreasing as k increasing. Our observed value z will be in the rejected region iff $z > k \Leftrightarrow \alpha > p^* = \mathbb{P}(Z > z \mid H_0)$.

Definition (p-value)**.** The quantity p^* is called the *p-value* of our observed data $\mathbf{x}$. For the example above, $z = 0.4$ and so $p^* = 1 - \Phi(0.4) = 0.3446$.

In general, the p-value is sometimes called the "observed significance level" of $\mathbf{x}$. This is the probability under H_0 of seeing data that is "more extreme" than our observed data $\mathbf{x}$. Extreme observations are viewed as providing evidence against H_0.

2.2 Composite hypotheses

For composite hypotheses like $H : \theta \geq 0$, the error probabilities do not have a single value. We define

Definition (Power function)**.** The *power function* is

$$W(\theta) = \mathbb{P}(\mathbf{X} \in C \mid \theta) = \mathbb{P}(\text{reject } H_0 \mid \theta),$$

We want $W(\theta)$ to be small on H_0 and large on H_1.

Definition (Size)**.** The *size* of the test is

$$\alpha = \sup_{\theta \in \Theta_0} W(\theta),$$

This is the worst possible size we can get.

For $\theta \in \Theta_1$, $1 - W(\theta) = \mathbb{P}(\text{Type II error} \mid \theta)$.

Sometimes the Neyman-Pearson theory can be extended to one-sided alternatives.

For example, in the previous example, we have shown that the most powerful size α test of $H_0 : \mu = \mu_0$ versus $H_1 : \mu = \mu_1$ (where $\mu_1 > \mu_0$) is given by

$$C = \left\{x : \frac{\sqrt{n}(\bar{x} - \mu_0)}{\sigma_0} > z_\alpha\right\}.$$

The critical region depends on $\mu_0, n, \sigma_0, \alpha$, and the fact that $\mu_1 > \mu_0$. It does *not* depend on the particular value of μ_1. This test is then uniformly the most powerful size α for testing $H_0 : \mu = \mu_0$ against $H_1 : \mu > \mu_0$.

Definition (Uniformly most powerful test)**.** A test specified by a critical region C is *uniformly most powerful* (UMP) size α test for test $H_0 : \theta \in \Theta_0$ against $H_1 : \theta \in \Theta_1$ if

(i) $\sup_{\theta \in \Theta_0} W(\theta) = \alpha$.

(ii) For any other test C^* with size $\leq \alpha$ and with power function W^*, we have $W(\theta) \geq W^*(\theta)$ for all $\theta \in \Theta_1$.

Note that these may not exist. However, the likelihood ratio test often works.

Example. Suppose $X_1, \cdots, X_n$ are iid $N(\mu, \sigma_0^2)$ where σ_0 is known, and we wish to test $H_0 : \mu \leq \mu_0$ against $H_1 : \mu > \mu_0$.

First consider testing $H_0' : \mu = \mu_0$ against $H_1' : \mu = \mu_1$, where $\mu_1 > \mu_0$. The Neyman-Pearson test of size α of H_0' against H_1' has

$$C = \left\{x : \frac{\sqrt{n}(\bar{x} - \mu_0)}{\sigma_0} > z_\alpha\right\}.$$

We show that C is in fact UMP for the composite hypotheses H_0 against H_1. For $\mu \in \mathbb{R}$, the power function is

$$\begin{aligned} W(\mu) &= \mathbb{P}_\mu(\text{reject } H_0) \\ &= \mathbb{P}_\mu\left(\frac{\sqrt{n}(\bar{X} - \mu_0)}{\sigma_0} > z_\alpha\right) \\ &= \mathbb{P}_\mu\left(\frac{\sqrt{n}(\bar{X} - \mu)}{\sigma_0} > z_\alpha + \frac{\sqrt{n}(\mu_0 - \mu)}{\sigma_0}\right) \\ &= 1 - \Phi\left(z_\alpha + \frac{\sqrt{n}(\mu_0 - \mu)}{\sigma_0}\right) \end{aligned}$$

To show this is UMP, we know that $W(\mu_0) = \alpha$ (by plugging in). $W(\mu)$ is an increasing function of μ. So

$$\sup_{\mu \leq \mu_0} W(\mu) = \alpha.$$

So the first condition is satisfied.

For the second condition, observe that for any $\mu > \mu_0$, the Neyman Pearson size α test of H_0' vs H_1' has critical region C. Let C^* and W^* belong to any other test of H_0 vs H_1 of size $\leq \alpha$. Then C^* can be regarded as a test of H_0' vs H_1' of size $\leq \alpha$, and the Neyman-Pearson lemma says that $W^*(\mu_1) \leq W(\mu_1)$. This holds for all $\mu_1 > \mu_0$. So the condition is satisfied and it is UMP.

We now consider likelihood ratio tests for more general situations.

Definition (Likelihood of a composite hypothesis)**.** The *likelihood* of a composite hypothesis $H : \theta \in \Theta$ given data $\mathbf{x}$ to be

$$L_{\mathbf{x}}(H) = \sup_{\theta \in \Theta} f(\mathbf{x} \mid \theta).$$

So far we have considered disjoint hypotheses Θ_0, Θ_1, but we are not interested in any specific alternative. So it is easier to take $\Theta_1 = \Theta$ rather than $\Theta \setminus \Theta_0$. Then

$$\Lambda_{\mathbf{x}}(H_0; H_1) = \frac{L_{\mathbf{x}}(H_1)}{L_{\mathbf{x}}(H_0)} = \frac{\sup_{\theta \in \Theta_1} f(\mathbf{x} \mid \theta)}{\sup_{\theta \in \Theta_0} f(\mathbf{x} \mid \theta)} \geq 1,$$

with large values of Λ indicating departure from H_0.

Example. Single sample: testing a given mean, known variance (z-test). Suppose that $X_1, \cdots, X_n$ are iid $N(\mu, \sigma_0^2)$, with σ_0^2 known, and we wish to test $H_0 : \mu = \mu_0$ against $H_1 : \mu \neq \mu_0$ (for given constant μ_0).

Here $\Theta_0 = \{\mu_0\}$ and $\Theta = \mathbb{R}$.

For the denominator, we have $\sup_\Theta f(\mathbf{x} \mid \mu) = f(\mathbf{x} \mid \hat{\mu})$, where $\hat{\mu}$ is the mle. We know that $\hat{\mu} = \bar{x}$. Hence

$$\Lambda_{\mathbf{x}}(H_0; H_1) = \frac{(2\pi\sigma_0^2)^{-n/2} \exp\left(-\frac{1}{2\sigma_0^2}\sum(x_i - \bar{x})^2\right)}{(2\pi\sigma_0^2)^{-n/2} \exp\left(-\frac{1}{2\sigma_0^2}\sum(x_i - \mu_0)^2\right)}.$$

Then H_0 is rejected if Λ_x is large.

To make our lives easier, we can use the logarithm instead:

$$2\log\Lambda(H_0; H_1) = \frac{1}{\sigma_0^2}\left[\sum(x_i - \mu_0)^2 - \sum(x_i - \bar{x})^2\right] = \frac{n}{\sigma_0^2}(\bar{x} - \mu_0)^2.$$

So we can reject H_0 if we have

$$\left|\frac{\sqrt{n}(\bar{x} - \mu_0)}{\sigma_0}\right| > c$$

for some c.

We know that under H_0, $Z = \dfrac{\sqrt{n}(\bar{X} - \mu_0)}{\sigma_0} \sim N(0, 1)$. So the size α generalised likelihood test rejects H_0 if

$$\left|\frac{\sqrt{n}(\bar{x} - \mu_0)}{\sigma_0}\right| > z_{\alpha/2}.$$

Alternatively, since $\dfrac{n(\bar{X} - \mu_0)}{\sigma_0^2} \sim \chi_1^2$, we reject H_0 if

$$\frac{n(\bar{X} - \mu_0)^2}{\sigma_0^2} > \chi_1^2(\alpha),$$

(check that $z_{\alpha/2}^2 = \chi_1^2(\alpha)$).

Note that this is a two-tailed test — i.e. we reject H_0 both for high and low values of $\bar{x}$.

The next theorem allows us to use likelihood ratio tests even when we cannot find the exact relevant null distribution.

First consider the "size" or "dimension" of our hypotheses: suppose that H_0 imposes p independent restrictions on Θ. So for example, if $\Theta = \{\theta : \theta = (\theta_1, \cdots, \theta_k)\}$, and we have

- $H_0 : \theta_{i_1} = a_1, \theta_{i_2} = a_2, \cdots \theta_{i_p} = a_p$; or
- $H_0 : A\theta = \mathbf{b}$ (with A $p \times k$, $\mathbf{b}$ $p \times 1$ given); or
- $H_0 : \theta_i = f_i(\varphi), i = 1, \cdots, k$ for some $\varphi = (\varphi_1, \cdots, \varphi_{k-p})$.

We say Θ has k free parameters and Θ_0 has $k - p$ free parameters. We write $|\Theta_0| = k - p$ and $|\Theta| = k$.

Theorem (Generalized likelihood ratio theorem)**.** Suppose $\Theta_0 \subseteq \Theta_1$ and $|\Theta_1| - |\Theta_0| = p$. Let $\mathbf{X} = (X_1, \cdots, X_n)$ with all X_i iid. Then if H_0 is true, as $n \to \infty$,

$$2 \log \Lambda_{\mathbf{X}}(H_0 : H_1) \sim \chi^2_p.$$

If H_0 is not true, then $2 \log \Lambda$ tends to be larger. We reject H_0 if $2 \log \Lambda > c$, where $c = \chi^2_p(\alpha)$ for a test of approximately size α.

For example, in our example above, $|\Theta_1| - |\Theta_0| = 1$, and in this case, we saw that under H_0, $2 \log \Lambda \sim \chi^2_1$ *exactly* for all n in that particular case, rather than just approximately.

2.3 Tests of goodness-of-fit and independence

2.3.1 Goodness-of-fit of a fully-specified null distribution

So far, we have considered relatively simple cases where we are attempting to figure out, say, the mean. However, in reality, more complicated scenarios arise. For example, we might want to know if a dice is fair, i.e. if the probability of getting each number is exactly $\frac{1}{6}$. Our null hypothesis would be that $p_1 = p_2 = \cdots = p_6 = \frac{1}{6}$, while the alternative hypothesis allows any possible values of p_i.

In general, suppose the observation space $\mathcal{X}$ is partitioned into k sets, and let p_i be the probability that an observation is in set i for $i = 1, \cdots, k$. We want to test "H_0 : the p_i's arise from a fully specified model" against "H_1 : the p_i's are unrestricted (apart from the obvious $p_i \geq 0, \sum p_i = 1$)".

Example. The following table lists the birth months of admissions to Oxford and Cambridge in 2012.

Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug
470	515	470	457	473	381	466	457	437	396	384	394

Is this compatible with a uniform distribution over the year?

Out of n independent observations, let N_i be the number of observations in ith set. So $(N_1, \cdots, N_k) \sim \text{multinomial}(n; p_1, \cdots, p_n)$.

For a generalized likelihood ratio test of H_0, we need to find the maximised likelihood under H_0 and H_1.

Under H_1, $\text{like}(p_1, \cdots, p_k) \propto p_1^{n_1} \cdots p_k^{n_k}$. So the log likelihood is $l = \text{constant} + \sum n_i \log p_i$. We want to maximise this subject to $\sum p_i = 1$. Using the Lagrange multiplier, we will find that the mle is $\hat{p_i} = n_i/n$. Also $|\Theta_1| = k - 1$ (not k, since they must sum up to 1).

Under H_0, the values of p_i are specified completely, say $p_i = \tilde{p}_i$. So $|\Theta_0| = 0$. Using our formula for $\hat{p_i}$, we find that

$$2 \log \Lambda = 2 \log \left(\frac{\hat{p}_1^{n_1} \cdots \hat{p}_k^{n_k}}{\tilde{p}_1^{n_1} \cdots \tilde{p}_k^{n_k}} \right) = 2 \sum n_i \log \left(\frac{n_i}{n \tilde{p}_i} \right) \tag{1}$$

Here $|\Theta_1| - |\Theta_0| = k - 1$. So we reject H_0 if $2 \log \Lambda > \chi^2_{k-1}(\alpha)$ for an approximate size α test.

Under H_0 (no effect of month of birth), $\tilde{p}_i$ is the proportion of births in month i in 1993/1994 — this is *not* simply proportional to the number of days in each month (or even worse, $\frac{1}{12}$), as there is for example an excess of September births (the "Christmas effect"). So

Then

$$2 \log \Lambda = 2 \sum n_i \log \left(\frac{n_i}{n \tilde{p}_i} \right) = 44.9.$$

$\mathbb{P}(\chi^2_{11} > 44.86) = 3 \times 10^{-9}$, which is our p-value. Since this is certainly less than 0.001, we can reject H_0 at the 0.1% level, or can say the result is "significant at the 0.1% level".

The traditional levels for comparison are $\alpha = 0.04, 0.01, 0.001$, roughly corresponding to "evidence", "strong evidence" and "very strong evidence".

A similar common situation has $H_0 : p_i = p_i(\theta)$ for some parameter θ and H_1 as before. Now $|\Theta_0|$ is the number of independent parameters to be estimated under H_0.

Under H_0, we find mle $\hat{\theta}$ by maximizing $n_i \log p_i(\theta)$, and then

$$2 \log \Lambda = 2 \log \left(\frac{\hat{p_1}^{n_1} \cdots \hat{p_k}^{n_k}}{p_1(\hat{\theta})^{n_1} \cdots p_k(\hat{\theta})^{n_1}} \right) = 2 \sum n_i \log \left(\frac{n_i}{n p_i(\hat{\theta})} \right). \tag{2}$$

The degrees of freedom are $k - 1 - |\Theta_0|$.

2.3.2 Pearson's Chi-squared test

Notice that the two log likelihoods are of the same form. In general, let $o_i = n_i$ (observed number) and let $e_i = n\tilde{p}_i$ or $np_i(\hat{\theta})$ (expected number). Let $\delta_i = o_i - e_i$. Then

$$\begin{aligned}
2 \log \Lambda &= 2 \sum o_i \log \left(\frac{o_i}{e_i} \right) \\
&= 2 \sum (e_i + \delta_i) \log \left(1 + \frac{\delta_i}{e_i} \right) \\
&= 2 \sum (e_i + \delta_i) \left(\frac{\delta_i}{e_i} - \frac{\delta_i^2}{2e_i^2} + O(\delta_i^3) \right) \\
&= 2 \sum \left(\delta_i + \frac{\delta_i^2}{e_i} - \frac{\delta_i^2}{2e_i} + O(\delta_i^3) \right)
\end{aligned}$$

We know that $\sum \delta_i = 0$ since $\sum e_i = \sum o_i$. So

$$\begin{aligned} &\approx \sum \frac{\delta_i^2}{e_i} \\ &= \sum \frac{(o_i - e_i)^2}{e_i}. \end{aligned}$$

This is known as the *Pearson's Chi-squared test*.

Example. Mendel crossed 556 smooth yellow male peas with wrinkled green peas. From the progeny, let

(i) N_1 be the number of smooth yellow peas,

(ii) N_2 be the number of smooth green peas,

(iii) N_3 be the number of wrinkled yellow peas,

(iv) N_4 be the number of wrinkled green peas.

We wish to test the goodness of fit of the model

$$H_0 : (p_1, p_2, p_3, p_4) = \left(\tfrac{9}{16}, \tfrac{3}{16}, \tfrac{3}{16}, \tfrac{1}{16}\right).$$

Suppose we observe $(n_1, n_2, n_3, n_4) = (315, 108, 102, 31)$.

We find $(e_1, e_2, e_3, e_4) = (312.75, 104.25, 104.25, 34.75)$. The actual $2 \log \Lambda = 0.618$ and the approximation we had is $\sum \frac{(o_i - e_i)^2}{e_i} = 0.604$.

Here $|\Theta_0| = 0$ and $|\Theta_1| = 4 - 1 = 3$. So we refer to test statistics $\chi^2_3(\alpha)$.

Since $\chi^2_3(0.05) = 7.815$, we see that neither value is significant at 5%. So there is no evidence against Mendel's theory. In fact, the p-value is approximately $\mathbb{P}(\chi^2_3 > 0.6) \approx 0.96$. This is a *really* good fit, so good that people suspect the numbers were not genuine.

Example. In a genetics problem, each individual has one of the three possible genotypes, with probabilities p_1, p_2, p_3. Suppose we wish to test $H_0 : p_i = p_i(\theta)$, where

$$p_1(\theta) = \theta^2, \quad p_2 = 2\theta(1 - \theta), \quad p_3(\theta) = (1 - \theta)^2.$$

for some $\theta \in (0, 1)$.

We observe $N_i = n_i$. Under H_0, the mle $\hat{\theta}$ is found by maximising

$$\sum n_i \log p_i(\theta) = 2n_1 \log \theta + n_2 \log(2\theta(1 - \theta)) + 2n_3 \log(1 - \theta).$$

We find that $\hat{\theta} = \frac{2n_1 + n_2}{2n}$. Also, $|\Theta_0| = 1$ and $|\Theta_1| = 2$.

After conducting an experiment, we can substitute $p_i(\hat{\theta})$ into (2), or find the corresponding Pearson's chi-squared statistic, and refer to χ^2_1.

2.3.3 Testing independence in contingency tables

Definition (Contingency table)**.** A *contingency table* is a table in which observations or individuals are classified according to one or more criteria.

Example. 500 people with recent car changes were asked about their previous and new cars. The results are as follows:

		New car		
		Large	Medium	Small
Previous car	Large	56	52	42
	Medium	50	83	67
	Small	18	51	81

This is a two-way contingency table: Each person is classified according to the previous car size and new car size.

Consider a two-way contingency table with r rows and c columns. For $i = 1, \cdots, r$ And $j = 1, \cdots, c$, let p_{ij} be the probability that an individual selected from the population under consideration is classified in row i and column j. (i.e. in the (i, j) cell of the table).

Let $p_{i+} = \mathbb{P}(\text{in row } i)$ and $p_{+j} = \mathbb{P}(\text{in column } j)$. Then we must have $p_{++} = \sum_i \sum_j p_{ij} = 1$.

Suppose a random sample of n individuals is taken, and let n_{ij} be the number of these classified in the (i, j) cell of the table.

Let $n_{i+} = \sum_j n_{ij}$ and $n_{+j} = \sum_i n_{ij}$. So $n_{++} = n$.

We have

$$(N_{11}, \cdots, N_{1c}, N_{21}, \cdots, N_{rc}) \sim \text{multinomial}(n; p_{11}, \cdots, p_{1c}, p_{21}, \cdots, p_{rc}).$$

We may be interested in testing the null hypothesis that the two classifications are independent. So we test

- H_0: $p_i = p_{i+}p_{+j}$ for all i, j, i.e. independence of columns and rows.
- H_1: p_{ij} are unrestricted.

Of course we have the usual restrictions like $p_{++} = 1$, $p_{ij} \geq 0$.

Under H_1, the mles are $\hat{p_{ij}} = \frac{n_{ij}}{n}$.

Under H_0, the mles are $\hat{p}_{i+} = \frac{n_{i+}}{n}$ and $\hat{p}_{+j} = \frac{n_{+j}}{n}$.

Write $o_{ij} = n_{ij}$ and $e_{ij} = n\hat{p}_{i+}\hat{p}_{+j} = n_{i+}n_{+j}/n$.

Then

$$2 \log \Lambda = 2 \sum_{i=1}^{r} \sum_{j=1}^{c} o_{ij} \log \left(\frac{o_{ij}}{e_{ij}} \right) \approx \sum_{i=1}^{r} \sum_{j=1}^{c} \frac{(o_{ij} - e_{ij})^2}{e_{ij}}.$$

using the same approximating steps for Pearson's Chi-squared test.

We have $|\Theta_1| = rc - 1$, because under H_1 the p_{ij}'s sum to one. Also, $|\Theta_0| = (r - 1) + (c - 1)$ because $p_{1+}, \cdots, p_{r+}$ must satisfy $\sum_i p_{i+} = 1$ and $p_{+1}, \cdots, p_{+c}$ must satisfy $\sum_j p_{+j} = 1$. So

$$|\Theta_1| - |\Theta_0| = rc - 1 - (r - 1) - (c - 1) = (r - 1)(c - 1).$$

Example. In our previous example, we wish to test H_0: the new and previous car sizes are independent. The actual data is:

		New car			
		Large	Medium	Small	**Total**
Previous car	Large	56	52	42	**150**
	Medium	50	83	67	**120**
	Small	18	51	81	**150**
	Total	*124*	*186*	*190*	***500***

while the expected values given by H_0 is

		New car			
		Large	Medium	Small	**Total**
Previous car	Large	37.2	55.8	57.0	**150**
	Medium	49.6	74.4	76.0	**120**
	Small	37.2	55.8	57.0	**150**
	Total	*124*	*186*	*190*	***500***

Note the margins are the same. It is quite clear that they do not match well, but we can find the p value to be sure.

$\sum\sum \frac{(o_{ij} - e_{ij})^2}{e_{ij}} = 36.20$, and the degrees of freedom is $(3-1)(3-1) = 4$.

From the tables, $\chi^2_4(0.05) = 9.488$ and $\chi^2_4(0.01) = 13.28$.

So our observed value of 36.20 is significant at the 1% level, i.e. there is strong evidence against H_0. So we conclude that the new and present car sizes are not independent.

2.4 Tests of homogeneity, and connections to confidence intervals

2.4.1 Tests of homogeneity

Example. 150 patients were randomly allocated to three groups of 50 patients each. Two groups were given a new drug at different dosage levels, and the third group received a placebo. The responses were as shown in the table below.

	Improved	No difference	Worse	**Total**
Placebo	18	17	15	**50**
Half dose	20	10	20	**50**
Full dose	25	13	12	**50**
Total	*63*	*40*	*47*	***150***

Here the row totals are fixed in advance, in contrast to our last section, where the row totals are random variables.

For the above, we may be interested in testing H_0 : the probability of "improved" is the same for each of the three treatment groups, and so are the probabilities of "no difference" and "worse", i.e. H_0 says that we have homogeneity down the rows.

In general, we have independent observations from r multinomial distributions, each of which has c categories, i.e. we observe an $r \times c$ table (n_{ij}), for $i = 1, \cdots, r$ and $j = 1, \cdots, c$, where

$$(N_{i1}, \cdots, N_{ic}) \sim \text{multinomial}(n_{i+}, p_{i1}, \cdots, p_{ic})$$

independently for each $i = 1, \cdots, r$. We want to test

$$H_0 : p_{1j} = p_{2j} = \cdots = p_{rj} = p_j,$$

for $j = 1, \cdots, c$, and

$$H_1 : p_{ij} \text{ are unrestricted.}$$

Using H_1,

$$\text{like}(p_{ij}) = \prod_{i=1}^{r} \frac{n_{i+}!}{n_{i1}! \cdots n_{ic}!} p_{i1}^{n_{i1}} \cdots p_{ic}^{n_{ic}},$$

and

$$\log \text{like} = \text{constant} + \sum_{i=1}^{r} \sum_{j=1}^{c} n_{ij} \log p_{ij}.$$

Using Lagrangian methods, we find that $\hat{p}_{ij} = \frac{n_{ij}}{n_{i+}}$.

Under H_0,

$$\log \text{like} = \text{constant} + \sum_{j=1}^{c} n_{+j} \log p_j.$$

By Lagrangian methods, we have $\hat{p}_j = \frac{n_{+j}}{n_{++}}$.

Hence

$$2 \log \Lambda = \sum_{i=1}^{r} \sum_{j=1}^{c} n_{ij} \log \left(\frac{\hat{p}_{ij}}{\hat{p}_j} \right) = 2 \sum_{i=1}^{r} \sum_{j=1}^{c} n_{ij} \log \left(\frac{n_{ij}}{n_{i+} n_{+j} / n_{++}} \right),$$

which is the same as what we had last time, when the row totals are unrestricted!

We have $|\Theta_1| = r(c-1)$ and $|\Theta_0| = c - 1$. So the degrees of freedom is $r(c-1) - (c-1) = (r-1)(c-1)$, and under H_0, $2 \log \Lambda$ is approximately $\chi^2_{(r-1)(c-1)}$. Again, it is exactly the same as what we had last time!

We reject H_0 if $2 \log \Lambda > \chi^2_{(r-1)(c-1)}(\alpha)$ for an approximate size α test.

If we let $o_{ij} = n_{ij}, e_{ij} = \frac{n_{i+} n_{+j}}{n_{++}}$, and $\delta_{ij} = o_{ij} - e_{ij}$, using the same approximating steps as for Pearson's Chi-squared, we obtain

$$2 \log \Lambda \approx \sum \frac{(o_{ij} - e_{ij})^2}{e_{ij}}.$$

Example. Continuing our previous example, our data is

	Improved	No difference	Worse	**Total**
Placebo	18	17	15	**50**
Half dose	20	10	20	**50**
Full dose	25	13	12	**50**
Total	*63*	*40*	*47*	***150***

The expected under H_0 is

	Improved	No difference	Worse	**Total**
Placebo	21	13.3	15.7	**50**
Half dose	21	13.3	15.7	**50**
Full dose	21	13.3	15.7	**50**
Total	*63*	*40*	*47*	***150***

We find $2\log\Lambda = 5.129$, and we refer this to χ^2_4. Clearly this is not significant, as the mean of χ^2_4 is 4, and is something we would expect to happen solely by chance.

We can calculate the p-value: from tables, $\chi^2_4(0.05) = 9.488$, so our observed value is not significant at 5%, and the data are consistent with H_0.

We conclude that there is no evidence for a difference between the drug at the given doses and the placebo.

For interest,

$$\sum \frac{(o_{ij} - e_{ij})^2}{e_{ij}} = 5.173,$$

giving the same conclusion.

2.4.2 Confidence intervals and hypothesis tests

Confidence intervals or sets can be obtained by inverting hypothesis tests, and vice versa

Definition (Acceptance region)**.** The *acceptance region* A of a test is the complement of the critical region C.

Note that when we say "acceptance", we really mean "non-rejection"! The name is purely for historical reasons.

Suppose $X_1, \cdots, X_n$ have joint pdf $f_{\mathbf{X}}(\mathbf{x} \mid \theta)$ for $\theta \in \Theta$

Theorem.

(i) Suppose that for every $\theta_0 \in \Theta$ there is a size α test of $H_0 : \theta = \theta_0$. Denote the acceptance region by $A(\theta_0)$. Then the set $I(\mathbf{X}) = \{\theta : \mathbf{X} \in A(\theta)\}$ is a $100(1-\alpha)\%$ confidence set for θ.

(ii) Suppose $I(\mathbf{X})$ is a $100(1-\alpha)\%$ confidence set for θ. Then $A(\theta_0) = \{\mathbf{X} : \theta_0 \in I(\mathbf{X})\}$ is an acceptance region for a size α test of $H_0 : \theta = \theta_0$.

Intuitively, this says that "confidence intervals" and "hypothesis acceptance/rejection" are the same thing. After gathering some data $\mathbf{X}$, we can produce a, say, 95% confidence interval (a, b). Then if we want to test the hypothesis $H_0 : \theta = \theta_0$, we simply have to check whether $\theta_0 \in (a, b)$.

On the other hand, if we have a test for $H_0 : \theta = \theta_0$, then the confidence interval is all θ_0 in which we would accept $H_0 : \theta = \theta_0$.

Proof. First note that $\theta_0 \in I(\mathbf{X})$ iff $\mathbf{X} \in A(\theta_0)$.

For (i), since the test is size α, we have

$$\mathbb{P}(\text{accept } H_0 \mid H_0 \text{ is true}) = \mathbb{P}(\mathbf{X} \in A_(\theta_0) \mid \theta = \theta_0) = 1 - \alpha.$$

And so

$$\mathbb{P}(\theta_0 \in I(\mathbf{X}) \mid \theta = \theta_0) = \mathbb{P}(\mathbf{X} \in A(\theta_0) \mid \theta = \theta_0) = 1 - \alpha.$$

For (ii), since $I(\mathbf{X})$ is a $100(1-\alpha)\%$ confidence set, we have

$$P(\theta_0 \in I(\mathbf{X}) \mid \theta = \theta_0) = 1 - \alpha.$$

So

$$\mathbb{P}(\mathbf{X} \in A(\theta_0) \mid \theta = \theta_0) = \mathbb{P}(\theta \in I(\mathbf{X}) \mid \theta = \theta_0) = 1 - \alpha. \qquad \square$$

Example. Suppose $X_1, \cdots, X_n$ are iid $N(\mu, 1)$ random variables and we want a 95% confidence set for μ.

One way is to use the theorem and find the confidence set that belongs to the hypothesis test that we found in the previous example. We find a test of size 0.05 of $H_0 : \mu = \mu_0$ against $H_1 : \mu \neq \mu_0$ that rejects H_0 when $|\sqrt{n}(\bar{x} - \mu_0)| > 1.96$ (where 1.96 is the upper 2.5% point of $N(0, 1)$).

Then $I(\mathbf{X}) = \{\mu : \mathbf{X} \in A(\mu)\} = \{\mu : |\sqrt{n}(\bar{X} - \mu)| < 1.96\%\}$. So a 95% confidence set for μ is $(\bar{X} - 1.96/\sqrt{n}, \bar{X} + 1.96/\sqrt{n})$.

2.5 Multivariate normal theory

2.5.1 Multivariate normal distribution

So far, we have only worked with scalar random variables or a vector of iid random variables. In general, we can have a random (column) vector $\mathbf{X} = (X_1, \cdots, X_n)^T$, where the X_i are correlated.

The mean of this vector is given by

$$\boldsymbol{\mu} = \mathbb{E}[\mathbf{X}] = (\mathbb{E}(X_1), \cdots, \mathbb{E}(X_n))^T = (\mu_1, \cdots, \mu_n)^T.$$

Instead of just the variance, we have the covariance matrix

$$\operatorname{cov}(\mathbf{X}) = \mathbb{E}[(\mathbf{X} - \boldsymbol{\mu})(\mathbf{X} - \boldsymbol{\mu})^T] = (\operatorname{cov}(X_i, X_j))_{ij},$$

provided they exist, of course.

We can multiply the vector $\mathbf{X}$ by an $m \times n$ matrix A. Then we have

$$\mathbb{E}[A\mathbf{X}] = A\boldsymbol{\mu},$$

and

$$\operatorname{cov}(A\mathbf{X}) = A \operatorname{cov}(\mathbf{X}) A^T. \qquad (*)$$

The last one comes from

$$\begin{aligned} \operatorname{cov}(A\mathbf{X}) &= \mathbb{E}[(A\mathbf{X} - \mathbb{E}[A\mathbf{X}])(A\mathbf{X} - \mathbb{E}[A\mathbf{X}])^T] \\ &= \mathbb{E}[A(\mathbf{X} - \mathbb{E}\mathbf{X})(\mathbf{X} - \mathbb{E}\mathbf{X})^T A^T] \\ &= A\mathbb{E}[(\mathbf{X} - \mathbb{E}\mathbf{X})(\mathbf{X} - \mathbb{E}\mathbf{X})^T] A^T. \end{aligned}$$

If we have two random vectors $\mathbf{V}, \mathbf{W}$, we can define the covariance $\operatorname{cov}(\mathbf{V}, \mathbf{W})$ to be a matrix with (i, j)th element $\operatorname{cov}(V_i, W_j)$. Then $\operatorname{cov}(A\mathbf{X}, B\mathbf{X}) = A \operatorname{cov}(\mathbf{X}) B^T$.

An important distribution is a *multivariate normal distribution*.

Definition (Multivariate normal distribution)**.** $\mathbf{X}$ has a *multivariate normal distribution* if, for every $\mathbf{t} \in \mathbb{R}^n$, the random variable $\mathbf{t}^T\mathbf{X}$ (i.e. $\mathbf{t} \cdot \mathbf{X}$) has a normal distribution. If $\mathbb{E}[\mathbf{X}] = \boldsymbol{\mu}$ and $\operatorname{cov}(\mathbf{X}) = \Sigma$, we write $\mathbf{X} \sim N_n(\boldsymbol{\mu}, \Sigma)$.

Note that Σ is symmetric and is positive semi-definite because by $(*)$,

$$\mathbf{t}^T \Sigma \mathbf{t} = \operatorname{var}(\mathbf{t}^T \mathbf{X}) \geq 0.$$

So what is the pdf of a multivariate normal? And what is the moment generating function? Recall that a (univariate) normal $X \sim N(\mu, \sigma^2)$ has density

$$f_X(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\frac{(x - \mu)^2}{\sigma^2}\right),$$

with moment generating function

$$M_X(s) = \mathbb{E}[e^{sX}] = \exp\left(\mu s + \frac{1}{2}\sigma^2 s^2\right).$$

Hence for any $\mathbf{t}$, the moment generating function of $\mathbf{t}^T\mathbf{X}$ is given by

$$M_{\mathbf{t}^T\mathbf{X}}(s) = \mathbb{E}[e^{s\mathbf{t}^T\mathbf{X}}] = \exp\left(\mathbf{t}^T\boldsymbol{\mu} s + \frac{1}{2}\mathbf{t}^T\Sigma\mathbf{t}s^2\right).$$

Hence $\mathbf{X}$ has mgf

$$M_{\mathbf{X}}(\mathbf{t}) = \mathbb{E}[e^{\mathbf{t}^T\mathbf{X}}] = M_{\mathbf{t}^T\mathbf{X}}(1) = \exp\left(\mathbf{t}^T\boldsymbol{\mu} + \frac{1}{2}\mathbf{t}^T\Sigma\mathbf{t}\right). \quad (\dagger)$$

Proposition.

(i) If $\mathbf{X} \sim N_n(\mu, \Sigma)$, and A is an $m \times n$ matrix, then $A\mathbf{X} \sim N_m(A\boldsymbol{\mu}, A\Sigma A^T)$.

(ii) If $\mathbf{X} \sim N_n(\mathbf{0}, \sigma^2 I)$, then

$$\frac{|\mathbf{X}|^2}{\sigma^2} = \frac{\mathbf{X}^T\mathbf{X}}{\sigma^2} = \sum \frac{X_i^2}{\sigma^2} \sim \chi_n^2.$$

Instead of writing $|\mathbf{X}|^2/\sigma^2 \sim \chi_n^2$, we often just say $|\mathbf{X}|^2 \sim \sigma^2\chi_n^2$.

Proof.

(i) See example sheet 3.

(ii) Immediate from definition of χ_n^2. □

Proposition. Let $\mathbf{X} \sim N_n(\mu, \Sigma)$. We split $\mathbf{X}$ up into two parts: $\mathbf{X} = \begin{pmatrix}\mathbf{X}_1\\ \mathbf{X}_2\end{pmatrix}$, where $\mathbf{X}_i$ is a $n_i \times 1$ column vector and $n_1 + n_2 = n$.

Similarly write

$$\boldsymbol{\mu} = \begin{pmatrix}\boldsymbol{\mu}_1\\ \boldsymbol{\mu}_2\end{pmatrix}, \quad \Sigma = \begin{pmatrix}\Sigma_{11} & \Sigma_{12}\\ \Sigma_{21} & \Sigma_{22}\end{pmatrix},$$

where Σ_{ij} is an $n_i \times n_j$ matrix.

Then

(i) $\mathbf{X}_i \sim N_{n_i}(\boldsymbol{\mu}_i, \Sigma_{ii})$

(ii) $\mathbf{X}_1$ and $\mathbf{X}_2$ are independent iff $\Sigma_{12} = 0$.

Proof.

(i) See example sheet 3.

(ii) Note that by symmetry of Σ, $\Sigma_{12} = 0$ if and only if $\Sigma_{21} = 0$.

From $(\dagger)$, $M_{\mathbf{X}}(\mathbf{t}) = \exp(\mathbf{t}^T\boldsymbol{\mu} + \frac{1}{2}\mathbf{t}^T\Sigma\mathbf{t})$ for each $\mathbf{t} \in \mathbb{R}^n$. We write $\mathbf{t} = \begin{pmatrix}\mathbf{t}_1\\ \mathbf{t}_2\end{pmatrix}$.

Then the mgf is equal to

$$M_{\mathbf{X}}(\mathbf{t}) = \exp\left(\mathbf{t}_1^T\boldsymbol{\mu}_1 + \mathbf{t}_2^T\Sigma_{11}\mathbf{t}_1 + \frac{1}{2}\mathbf{t}_2^T\Sigma_{22}\mathbf{t}_2 + \frac{1}{2}\mathbf{t}_1^T\Sigma_{12}\mathbf{t}_2 + \frac{1}{2}\mathbf{t}_2^T\Sigma_{21}\mathbf{t}_1\right).$$

From (i), we know that $M_{\mathbf{X}_i}(\mathbf{t}_i) = \exp(\mathbf{t}_i^T\boldsymbol{\mu}_i + \frac{1}{2}\mathbf{t}_i^T\Sigma_{ii}\mathbf{t}_i)$. So $M_{\mathbf{X}}(\mathbf{t}) = M_{\mathbf{X}_1}(\mathbf{t}_1)M_{\mathbf{X}_2}(\mathbf{t}_2)$ for all $\mathbf{t}$ if and only if $\Sigma_{12} = 0$. □

Proposition. When Σ is a positive definite, then $\mathbf{X}$ has pdf

$$f_{\mathbf{X}}(\mathbf{x}; \mu, \Sigma) = \frac{1}{|\Sigma|^2}\left(\frac{1}{\sqrt{2\pi}}\right)^n \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right].$$

Note that Σ is always positive semi-definite. The conditions just forbid the case $|\Sigma| = 0$, since this would lead to dividing by zero.

2.5.2 Normal random samples

We wish to use our knowledge about multivariate normals to study univariate normal data. In particular, we want to prove the following:

Theorem (Joint distribution of $\bar{X}$ and S_{XX})**.** Suppose $X_1, \cdots, X_n$ are iid $N(\mu, \sigma^2)$ and $\bar{X} = \frac{1}{n}\sum X_i$, and $S_{XX} = \sum (X_i - \bar{X})^2$. Then

(i) $\bar{X} \sim N(\mu, \sigma^2/n)$

(ii) $S_{XX}/\sigma^2 \sim \chi^2_{n-1}$.

(iii) $\bar{X}$ and S_{XX} are independent.

Proof. We can write the joint density as $\mathbf{X} \sim N_n(\boldsymbol{\mu}, \sigma^2 I)$, where $\boldsymbol{\mu} = (\mu, \mu, \cdots, \mu)$.

Let A be an $n \times n$ orthogonal matrix with the first row all $1/\sqrt{n}$ (the other rows are not important). One possible such matrix is

$$A = \begin{pmatrix} \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \cdots & \frac{1}{\sqrt{n}} \\ \frac{1}{\sqrt{2\times 1}} & \frac{-1}{\sqrt{2\times 1}} & 0 & 0 & \cdots & 0 \\ \frac{1}{\sqrt{3\times 2}} & \frac{1}{\sqrt{3\times 2}} & \frac{-2}{\sqrt{3\times 2}} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \frac{1}{\sqrt{n(n-1)}} & \cdots & \frac{-(n-1)}{\sqrt{n(n-1)}} \end{pmatrix}$$

Now define $\mathbf{Y} = A\mathbf{X}$. Then

$$\mathbf{Y} \sim N_n(A\boldsymbol{\mu}, A\sigma^2 I A^T) = N_n(A\boldsymbol{\mu}, \sigma^2 I).$$

We have

$$A\boldsymbol{\mu} = (\sqrt{n}\mu, 0, \cdots, 0)^T.$$

So $Y_1 \sim N(\sqrt{n}\mu, \sigma^2)$ and $Y_i \sim N(0, \sigma^2)$ for $i = 2, \cdots, n$. Also, $Y_1, \cdots, Y_n$ are independent, since the covariance matrix is every non-diagonal term 0.

But from the definition of A, we have

$$Y_1 = \frac{1}{\sqrt{n}}\sum_{i=1}^n X_i = \sqrt{n}\bar{X}.$$

So $\sqrt{n}\bar{X} \sim N(\sqrt{n}\mu, \sigma^2)$, or $\bar{X} \sim N(\mu, \sigma^2/n)$. Also

$$\begin{aligned} Y_2^2 + \cdots + Y_n^2 &= \mathbf{Y}^T\mathbf{Y} - Y_1^2 \\ &= \mathbf{X}^T A^T A \mathbf{X} - Y_1^2 \\ &= \mathbf{X}^T\mathbf{X} - n\bar{X}^2 \\ &= \sum_{i=1}^n X_i^2 - n\bar{X}^2 \\ &= \sum_{i=1}^n (X_i - \bar{X})^2 \\ &= S_{XX}. \end{aligned}$$

So $S_{XX} = Y_2^2 + \cdots + Y_n^2 \sim \sigma^2\chi^2_{n-1}$.

Finally, since Y_1 and $Y_2, \cdots, Y_n$ are independent, so are $\bar{X}$ and S_{XX}. □

2.6 Student's t-distribution

Definition (t-distribution)**.** Suppose that Z and Y are independent, $Z \sim N(0,1)$ and $Y \sim \chi^2_k$. Then

$$T = \frac{Z}{\sqrt{Y/k}}$$

is said to have a t-distribution on k degrees of freedom, and we write $T \sim t_k$.

The density of t_k turns out to be

$$f_T(t) = \frac{\Gamma((k+1)/2)}{\Gamma(k/2)} \frac{1}{\sqrt{\pi k}} \left(1 + \frac{t^2}{k}\right)^{-(k+1)/2}.$$

This density is symmetric, bell-shaped, and has a maximum at $t = 0$, which is rather like the standard normal density. However, it can be shown that $\mathbb{P}(T > t) > \mathbb{P}(Z > t)$, i.e. the T distribution has a "fatter" tail. Also, as $k \to \infty$, t_k approaches a normal distribution.

Proposition. If $k > 1$, then $\mathbb{E}_k(T) = 0$.

If $k > 2$, then $\mathrm{var}_k(T) = \frac{k}{k-2}$.

If $k = 2$, then $\mathrm{var}_k(T) = \infty$.

In all other cases, the values are undefined. In particular, the $k = 1$ case, this is known as the Cauchy distribution, and has undefined mean and variance.

Notation. We write $t_k(\alpha)$ be the upper $100\alpha\%$ point of the t_k distribution, so that $\mathbb{P}(T > t_k(\alpha)) = \alpha$.

Why would we define such a weird distribution? The typical application is to study random samples with unknown mean *and* unknown variance.

Let $X_1, \cdots, X_n$ be iid $\mathbb{N}(\mu, \sigma^2)$. Then $\bar{X} \sim N(\mu, \sigma^2/n)$. So $Z = \frac{\sqrt{n}(\bar{X}-\mu)}{\sigma} \sim N(0,1)$.

Also, $S_{XX}/\sigma^2 \sim \chi^2_{n-1}$ and is independent of $\bar{X}$, and hence Z. So

$$\frac{\sqrt{n}(\bar{X} - \mu)/\sigma}{\sqrt{S_{XX}/((n-1)\sigma^2)}} \sim t_{n-1},$$

or

$$\frac{\sqrt{n}(\bar{X}-\mu)}{\sqrt{S_{XX}/(n-1)}} \sim t_{n-1}.$$

We write $\tilde{\sigma}^2 = \frac{S_{XX}}{n-1}$ (note that this is the unbiased estimator). Then a $100(1-\alpha)\%$ confidence interval for μ is found from

$$1-\alpha = \mathbb{P}\left(-t_{n-1}\left(\frac{\alpha}{2}\right) \leq \frac{\sqrt{n}(\bar{X}-\mu)}{\tilde{\sigma}} \leq t_{n-1}\left(\frac{\alpha}{2}\right)\right).$$

This has endpoints

$$\bar{X} \pm \frac{\tilde{\sigma}}{\sqrt{n}} t_{n-1}\left(\frac{\alpha}{2}\right).$$

3 Linear models

3.1 Linear models

Linear models can be used to explain or model the relationship between a *response* (or *dependent*) variable, and one or more *explanatory* variables (or *covariates* or *predictors*). As the name suggests, we assume the relationship is linear.

Example. How do motor insurance claim rates (response) depend on the age and sex of the driver, and where they live (explanatory variables)?

It is important to note that (unless otherwise specified), we do *not* assume normality in our calculations here.

Suppose we have p covariates x_j, and we have n observations Y_i. We assume $n > p$, or else we can pick the parameters to fix our data exactly. Then each observation can be written as

$$Y_i = \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \varepsilon_i. \qquad ((*))$$

for $i = 1, \cdots, n$. Here

- $\beta_1, \cdots, \beta_p$ are unknown, fixed parameters we wish to work out (with $n > p$)
- $x_{i1}, \cdots, x_{ip}$ are the values of the p covariates for the ith response (which are all known).
- $\varepsilon_1, \cdots, \varepsilon_n$ are independent (or possibly just uncorrelated) random variables with mean 0 and variance σ^2.

We think of the $\beta_j x_{ij}$ terms to be the causal effects of x_{ij} and ε_i to be a random fluctuation (error term).

Then we clearly have

- $\mathbb{E}(Y_i) = \beta_1 x_{i1} + \cdots \beta_p x_{ip}$.
- $\text{var}(Y_i) = \text{var}(\varepsilon_i) = \sigma^2$.
- $Y_1, \cdots, Y_n$ are independent.

Note that $(*)$ is linear in the parameters $\beta_1, \cdots, \beta_p$. Obviously the real world can be much more complicated. But this is much easier to work with.

Example. For each of 24 males, the maximum volume of oxygen uptake in the blood and the time taken to run 2 miles (in minutes) were measured. We want to know how the time taken depends on oxygen uptake.

We might get the results

Oxygen	42.3	53.1	42.1	50.1	42.5	42.5	47.8	49.9
Time	918	805	892	962	968	907	770	743
Oxygen	36.2	49.7	41.5	46.2	48.2	43.2	51.8	53.3
Time	1045	810	927	813	858	860	760	747
Oxygen	53.3	47.2	56.9	47.8	48.7	53.7	60.6	56.7
Time	743	803	683	844	755	700	748	775

For each individual i, we let Y_i be the time to run 2 miles, and x_i be the maximum volume of oxygen uptake, $i = 1, \cdots, 24$. We might want to fit a straight line to it. So a possible model is

$$Y_i = a + bx_i + \varepsilon_i,$$

where ε_i are independent random variables with variance σ^2, and a and b are constants.

The subscripts in the equation makes it tempting to write them as matrices:

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix}, \quad X = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{np}. \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}, \quad \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

Then the equation becomes

$$\mathbf{Y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}. \tag{2}$$

We also have

- $\mathbb{E}(\boldsymbol{\varepsilon}) = \mathbf{0}$.
- $\operatorname{cov}(\mathbf{Y}) = \sigma^2 I$.

We assume throughout that X has full rank p, i.e. the columns are independent, and that the error variance is the same for each observation. We say this is the *homoscedastic* case, as opposed to *heteroscedastic*.

Example. Continuing our example, we have, in matrix form

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ \vdots \\ Y_{24} \end{pmatrix}, \quad X = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_{24} \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} a \\ b \end{pmatrix}, \quad \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_{24}. \end{pmatrix}$$

Then

$$\mathbf{Y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}.$$

Definition (Least squares estimator)**.** In a linear model $\mathbf{Y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, the *least squares estimator* $\hat{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}$ minimizes

$$\begin{aligned} S(\boldsymbol{\beta}) &= \|\mathbf{Y} - X\boldsymbol{\beta}\|^2 \\ &= (\mathbf{Y} - X\boldsymbol{\beta})^T(\mathbf{Y} - X\boldsymbol{\beta}) \\ &= \sum_{i=1}^{n} (Y_i - x_{ij}\beta_j)^2 \end{aligned}$$

with implicit summation over j.

If we plot the points on a graph, then the least square estimators minimizes the (square of the) vertical distance between the points and the line.

To minimize it, we want

$$\left.\frac{\partial S}{\partial \beta_k}\right|_{\boldsymbol{\beta}=\hat{\boldsymbol{\beta}}} = 0$$

for all k. So

$$-2x_{ik}(Y_i - x_{ij}\hat{\beta}_j) = 0$$

for each k (with implicit summation over i and j), i.e.

$$x_{ik}x_{ij}\hat{\beta}_j = x_{ik}Y_i$$

for all k. Putting this back in matrix form, we have

Proposition. The least squares estimator satisfies

$$X^TX\hat{\boldsymbol{\beta}} = X^T\mathbf{Y}. \tag{3}$$

We could also have derived this by completing the square of $(\mathbf{Y} - X\boldsymbol{\beta})^T(\mathbf{Y} - X\boldsymbol{\beta})$, but that would be more complicated.

In order to find $\hat{\boldsymbol{\beta}}$, our life would be much easier if X^TX has an inverse. Fortunately, it always does. We assumed that X is of full rank p. Then

$$\mathbf{t}X^TX\mathbf{t} = (X\mathbf{t})^T(X\mathbf{t}) = \|X\mathbf{t}\|^2 > 0$$

for $\mathbf{t} \neq \mathbf{0}$ in $\mathbb{R}^p$ (the last inequality is since if there were a $\mathbf{t}$ such that $\|X\mathbf{t}\| = 0$, then we would have produced a linear combination of the columns of X that gives $\mathbf{0}$). So X^TX is positive definite, and hence has an inverse. So

$$\hat{\boldsymbol{\beta}} = (X^TX)^{-1}X^T\mathbf{Y}, \tag{4}$$

which is linear in $\mathbf{Y}$.

We have

$$\mathbb{E}(\hat{\boldsymbol{\beta}}) = (X^TX^{-1})X^T\mathbb{E}[\mathbf{Y}] = (X^TX)^{-1}X^TX\boldsymbol{\beta} = \boldsymbol{\beta}.$$

So $\hat{\boldsymbol{\beta}}$ is an unbiased estimator for $\boldsymbol{\beta}$. Also

$$\operatorname{cov}(\hat{\boldsymbol{\beta}}) = (X^TX)^{-1}X^T\operatorname{cov}(\mathbf{Y})X(X^TX)^{-1} = \sigma^2(X^TX)^{-1}, \tag{5}$$

since $\operatorname{cov}\mathbf{Y} = \sigma^2 I$.

3.2 Simple linear regression

What we did above was *so* complicated. If we have a simple linear regression model

$$Y_i = a + bx_i + \varepsilon_i.$$

then we can reparameterise it to

$$Y_i = a' + b(x_i - \bar{x}) + \varepsilon_i, \tag{6}$$

where $\bar{x} = \sum x_i/n$ and $a' = a + b\bar{x}$. Since $\sum(x_i - \bar{x}) = 0$, this leads to simplified calculations.

In matrix form,

$$X = \begin{pmatrix} 1 & (x_1 - \bar{x}) \\ \vdots & \vdots \\ 1 & (x_{24} - \bar{x}) \end{pmatrix}.$$

Since $\sum(x_i - \bar{x}) = 0$, in X^TX, the off-diagonals are all 0, and we have

$$X^TX = \begin{pmatrix} n & 0 \\ 0 & S_{xx} \end{pmatrix},$$

where $S_{xx} = \sum (x_i - \bar{x})^2$.

Hence

$$(X^T X)^{-1} = \begin{pmatrix} \frac{1}{n} & 0 \\ 0 & \frac{1}{S_{xx}} \end{pmatrix}$$

So

$$\hat{\boldsymbol{\beta}} = (X^T X^{-1}) X^T \mathbf{Y} = \begin{pmatrix} \bar{Y} \\ \frac{S_{xY}}{S_{xx}} \end{pmatrix},$$

where $S_{xY} = \sum Y_i (x_i - \bar{x})$.

Hence the estimated intercept is $\hat{a}' = \bar{y}$, and the estimated gradient is

$$\begin{aligned} \hat{b} &= \frac{S_{xy}}{S_{xx}} \\ &= \frac{\sum_i y_i (x_i - \bar{x})}{\sum_i (x_i - \bar{x})^2} \\ &= \frac{\sum_i (y_i - \bar{y})(x_i - \bar{x})}{\sqrt{\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2}} \times \sqrt{\frac{S_{yy}}{S_{xx}}} \qquad (*) \\ &= r \times \sqrt{\frac{S_{yy}}{S_{xx}}}. \end{aligned}$$

We have $(*)$ since $\sum \bar{y}(x_i - \bar{x}) = 0$, so we can add it to the nominator. Then the other square root things are just multiplying and dividing by the same things.

So the gradient is the *Pearson product-moment correlation coefficient* r times the ratio of the empirical standard deviations of the y's and x's (note that the gradient is the same whether the x's are standardised to have mean 0 or not).

Hence we get $\text{cov}(\hat{\boldsymbol{\beta}}) = (X^T X)^{-1} \sigma^2$, and so from our expression of $(X^T X)^{-1}$,

$$\text{var}(\hat{a}') = \text{var}(\bar{Y}) = \frac{\sigma^2}{n}, \quad \text{var}(\hat{b}) = \frac{\sigma^2}{S_{xx}}.$$

Note that these estimators are uncorrelated.

Note also that these are obtained without any explicit distributional assumptions.

Example. Continuing our previous oxygen/time example, we have $\bar{y} = 826.5$, $S_{xx} = 783.5 = 28.0^2$, $S_{xy} = -10077$, $S_{yy} = 444^2$, $r = -0.81$, $\hat{b} = -12.9$.

Theorem (Gauss Markov theorem)**.** In a full rank linear model, let $\hat{\boldsymbol{\beta}}$ be the least squares estimator of $\boldsymbol{\beta}$ and let $\boldsymbol{\beta}^*$ be any other unbiased estimator for $\boldsymbol{\beta}$ which is linear in the Y_i's. Then

$$\text{var}(\mathbf{t}^T \hat{\boldsymbol{\beta}}) \leq \text{var}(\mathbf{t}^T \boldsymbol{\beta}^*).$$

for all $\mathbf{t} \in \mathbb{R}^p$. We say that $\hat{\boldsymbol{\beta}}$ is the *best linear unbiased estimator* of $\boldsymbol{\beta}$ (BLUE).

Proof. Since $\boldsymbol{\beta}^*$ is linear in the Y_i's, $\boldsymbol{\beta}^* = A\mathbf{Y}$ for some $p \times n$ matrix A.

Since $\boldsymbol{\beta}^*$ is an unbiased estimator, we must have $\mathbb{E}[\boldsymbol{\beta}^*] = \boldsymbol{\beta}$. However, since $\boldsymbol{\beta}^* = A\mathbf{Y}$, $\mathbb{E}[\boldsymbol{\beta}^*] = A\mathbb{E}[\mathbf{Y}] = AX\boldsymbol{\beta}$. So we must have $\boldsymbol{\beta} = AX\boldsymbol{\beta}$. Since this holds for any $\boldsymbol{\beta}$, we must have $AX = I_p$. Now

$$\begin{aligned} \text{cov}(\boldsymbol{\beta}^*) &= \mathbb{E}[(\boldsymbol{\beta}^* - \boldsymbol{\beta})(\boldsymbol{\beta}^* - \boldsymbol{\beta})^T] \\ &= \mathbb{E}[(A\mathbf{Y} - \boldsymbol{\beta})(A\mathbf{Y} - \boldsymbol{\beta})^T] \\ &= \mathbb{E}[(AX\boldsymbol{\beta} + A\boldsymbol{\varepsilon} - \boldsymbol{\beta})(AX\boldsymbol{\beta} + A\boldsymbol{\varepsilon} - \boldsymbol{\beta})^T] \end{aligned}$$

Since $AX\boldsymbol{\beta} = \boldsymbol{\beta}$, this is equal to

$$\begin{aligned} &= \mathbb{E}[A\boldsymbol{\varepsilon}(A\boldsymbol{\varepsilon})^T] \\ &= A(\sigma^2 I)A^T \\ &= \sigma^2 AA^T. \end{aligned}$$

Now let $\boldsymbol{\beta}^* - \hat{\boldsymbol{\beta}} = (A - (X^TX)^{-1}X^T)\mathbf{Y} = B\mathbf{Y}$, for some B. Then

$$BX = AX - (X^TX^{-1})X^TX = I_p - I_p = 0.$$

By definition, we have $A\mathbf{Y} = B\mathbf{Y} + (X^TX)^{-1}X^T\mathbf{Y}$, and this is true for all $\mathbf{Y}$. So $A = B + (X^TX)^{-1}X^T$. Hence

$$\begin{aligned} \operatorname{cov}(\boldsymbol{\beta}^*) &= \sigma^2 AA^T \\ &= \sigma^2(B + (X^TX)^{-1}X^T)(B + (X^TX)^{-1}X^T)^T \\ &= \sigma^2(BB^T + (X^TX)^{-1}) \\ &= \sigma^2 BB^T + \operatorname{cov}(\hat{\boldsymbol{\beta}}). \end{aligned}$$

Note that in the second line, the cross-terms disappear since $BX = 0$.

So for any $\mathbf{t} \in \mathbb{R}^p$, we have

$$\begin{aligned} \operatorname{var}(\mathbf{t}^T\boldsymbol{\beta}^*) &= \mathbf{t}^T \operatorname{cov}(\boldsymbol{\beta}^*)\mathbf{t} \\ &= \mathbf{t}^T \operatorname{cov}(\hat{\boldsymbol{\beta}})\mathbf{t} + \mathbf{t}^T BB^T\mathbf{t}\sigma^2 \\ &= \operatorname{var}(\mathbf{t}^T\hat{\boldsymbol{\beta}}) + \sigma^2\|B^T\mathbf{t}\|^2 \\ &\geq \operatorname{var}(\mathbf{t}^T\hat{\boldsymbol{\beta}}). \end{aligned}$$

Taking $\mathbf{t} = (0, \cdots, 1, 0, \cdots, 0)^T$ with a 1 in the ith position, we have

$$\operatorname{var}(\hat{\beta}_i) \leq \operatorname{var}(\beta_i^*). \qquad \square$$

Definition (Fitted values and residuals)**.** $\hat{\mathbf{Y}} = X\hat{\boldsymbol{\beta}}$ is the *vector of fitted values*. These are what our model says $\mathbf{Y}$ should be.

$\mathbf{R} = \mathbf{Y} - \hat{\mathbf{Y}}$ is the *vector of residuals*. These are the deviations of our model from reality.

The *residual sum of squares* is

$$\text{RSS} = \|\mathbf{R}\|^2 = \mathbf{R}^T\mathbf{R} = (\mathbf{Y} - X\hat{\boldsymbol{\beta}})^T(\mathbf{Y} - X\hat{\boldsymbol{\beta}}).$$

We can give these a geometric interpretation. Note that $X^T\mathbf{R} = X^T(\mathbf{Y} - \hat{\mathbf{Y}}) = X^T\mathbf{Y} - X^TX\hat{\boldsymbol{\beta}} = 0$ by our formula for $\boldsymbol{\beta}$. So $\mathbf{R}$ is orthogonal to the column space of X.

Write $\hat{\mathbf{Y}} = X\hat{\boldsymbol{\beta}} = X(X^TX)^{-1}X^T\mathbf{Y} = P\mathbf{Y}$, where $P = X(X^TX)^{-1}X^T$. Then P represents an orthogonal projection of $\mathbb{R}^n$ onto the space spanned by the columns of X, i.e. it projects the actual data $\mathbf{Y}$ to the fitted values $\hat{\mathbf{Y}}$. Then $\mathbf{R}$ is the part of $\mathbf{Y}$ orthogonal to the column space of X.

The projection matrix P is idempotent and symmetric, i.e. $P^2 = P$ and $P^T = P$.

3.3 Linear models with normal assumptions

So far, we have not assumed anything about our variables. In particular, we have not assumed that they are normal. So what further information can we obtain by assuming normality?

Example. Suppose we want to measure the resistivity of silicon wafers. We have five instruments, and five wafers were measured by each instrument (so we have 25 wafers in total). We assume that the silicon wafers are all the same, and want to see whether the instruments consistent with each other, i.e. The results are as follows:

		Wafer				
		1	2	3	4	5
Instrument	1	130.5	112.4	118.9	125.7	134.0
	2	130.4	138.2	116.7	132.6	104.2
	3	113.0	120.5	128.9	103.4	118.1
	4	128.0	117.5	114.9	114.9	98.8
	5	121.2	110.5	118.5	100.5	120.9

Let $Y_{i,j}$ be the resistivity of the jth wafer measured by instrument i, where $i, j = 1, \cdots, 5$. A possible model is

$$Y_{i,j} = \mu_i + \varepsilon_{i,j},$$

where ε_{ij} are independent random variables such that $\mathbb{E}[\varepsilon_{ij}] = 0$ and $\text{var}(\varepsilon_{ij}) = \sigma^2$, and the μ_i's are unknown constants.

This can be written in matrix form, with

$$\mathbf{Y} = \begin{pmatrix} Y_{1,1} \\ \vdots \\ Y_{1,5} \\ Y_{2,1} \\ \vdots \\ Y_{2,5} \\ \vdots \\ Y_{5,1} \\ \vdots \\ Y_{5,5} \end{pmatrix}, \quad X = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \end{pmatrix}, \quad \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{1,1} \\ \vdots \\ \varepsilon_{1,5} \\ \varepsilon_{2,1} \\ \vdots \\ \varepsilon_{2,5} \\ \vdots \\ \varepsilon_{5,1} \\ \vdots \\ \varepsilon_{5,5} \end{pmatrix}$$

Then

$$\mathbf{Y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}.$$

We have

$$X^T X = \begin{pmatrix} 5 & 0 & \cdots & 0 \\ 0 & 5 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 5 \end{pmatrix}$$

Hence

$$(X^TX)^{-1} = \begin{pmatrix} \frac{1}{5} & 0 & \cdots & 0 \\ 0 & \frac{1}{5} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{5} \end{pmatrix}$$

So we have

$$\hat{\boldsymbol{\mu}} = (X^TX)^{-1}X^T\mathbf{Y} = \begin{pmatrix} \bar{Y}_1 \\ \vdots \\ \bar{Y}_5 \end{pmatrix}$$

The residual sum of squares is

$$\text{RSS} = \sum_{i=1}^{5}\sum_{j=1}^{5}(Y_{i,j} - \hat{\mu}_i)^2 = \sum_{i=1}^{5}\sum_{j=1}^{5}(Y_{i,j} - \bar{Y}_i)^2 = 2170.$$

This has $n - p = 25 - 5 = 20$ degrees of freedom. We will later see that $\bar{\sigma} = \sqrt{\text{RSS}/(n-p)} = 10.4$.

Note that we still haven't used normality!

We now make a normal assumption:

$$\mathbf{Y} = X\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim N_n(\mathbf{0}, \sigma^2 I), \quad \text{rank}(X) = p < n.$$

This is a special case of the linear model we just had, so all previous results hold.

Since $\mathbf{Y} = N_n(X\boldsymbol{\beta}, \sigma^2 I)$, the log-likelihood is

$$l(\boldsymbol{\beta}, \sigma^2) = -\frac{n}{2}\log 2\pi - \frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2}S(\boldsymbol{\beta}),$$

where

$$S(\boldsymbol{\beta}) = (\mathbf{Y} - X\boldsymbol{\beta})^T(\mathbf{Y} - X\boldsymbol{\beta}).$$

If we want to maximize l with respect to $\boldsymbol{\beta}$, we have to maximize the only term containing $\boldsymbol{\beta}$, i.e. $S(\boldsymbol{\beta})$. So

Proposition. Under normal assumptions the maximum likelihood estimator for a linear model is

$$\hat{\boldsymbol{\beta}} = (X^TX)^{-1}X^T\mathbf{Y},$$

which is the same as the least squares estimator.

This isn't coincidence! Historically, when Gauss devised the normal distribution, he designed it so that the least squares estimator is the same as the maximum likelihood estimator.

To obtain the MLE for σ^2, we require

$$\left.\frac{\partial l}{\partial \sigma^2}\right|_{\hat{\boldsymbol{\beta}}, \hat{\sigma}^2} = 0,$$

i.e.

$$-\frac{n}{2\sigma^2} + \frac{S(\hat{\boldsymbol{\beta}})}{2\hat{\sigma}^4} = 0$$

So

$$\hat{\sigma}^2 = \frac{1}{n}S(\hat{\boldsymbol{\beta}}) = \frac{1}{n}(\mathbf{Y} - X\hat{\boldsymbol{\beta}})^T(\mathbf{Y} - X\hat{\boldsymbol{\beta}}) = \frac{1}{n}\text{RSS}.$$

Our ultimate goal now is to show that $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}^2$ are independent. Then we can apply our other standard results such as the t-distribution.

First recall that the matrix $P = X(X^TX)^{-1}X^T$ that projects $\mathbf{Y}$ to $\hat{\mathbf{Y}}$ is idempotent and symmetric. We will prove the following properties of it:

Lemma.

(i) If $\mathbf{Z} \sim N_n(\mathbf{0}, \sigma^2 I)$ and A is $n \times n$, symmetric, idempotent with rank r, then $\mathbf{Z}^T A\mathbf{Z} \sim \sigma^2\chi^2_r$.

(ii) For a symmetric idempotent matrix A, $\text{rank}(A) = \text{tr}(A)$.

Proof.

(i) Since A is idempotent, $A^2 = A$ by definition. So eigenvalues of A are either 0 or 1 (since $\lambda\mathbf{x} = A\mathbf{x} = A^2\mathbf{x} = \lambda^2\mathbf{x}$).

Since A is also symmetric, it is diagonalizable. So there exists an orthogonal Q such that

$$\Lambda = Q^TAQ = \text{diag}(\lambda_1, \cdots, \lambda_n) = \text{diag}(1, \cdots, 1, 0, \cdots, 0)$$

with r copies of 1 and $n - r$ copies of 0.

Let $\mathbf{W} = Q^T\mathbf{Z}$. So $\mathbf{Z} = Q\mathbf{W}$. Then $\mathbf{W} \sim N_n(\mathbf{0}, \sigma^2 I)$, since $\text{cov}(\mathbf{W}) = Q^T\sigma^2 IQ = \sigma^2 I$. Then

$$\mathbf{Z}^T A\mathbf{Z} = \mathbf{W}^T Q^T AQ\mathbf{W} = \mathbf{W}^T\Lambda\mathbf{W} = \sum_{i=1}^{r} w_i^2 \sim \chi^2_r.$$

(ii)

$$\begin{aligned}\text{rank}(A) &= \text{rank}(\Lambda)\\ &= \text{tr}(\Lambda)\\ &= \text{tr}(Q^TAQ)\\ &= \text{tr}(AQ^TQ)\\ &= \text{tr}\, A\end{aligned}$$

□

Theorem. For the normal linear model $\mathbf{Y} \sim N_n(X\boldsymbol{\beta}, \sigma^2 I)$,

(i) $\hat{\boldsymbol{\beta}} \sim N_p(\boldsymbol{\beta}, \sigma^2(X^TX)^{-1})$

(ii) $\text{RSS} \sim \sigma^2\chi^2_{n-p}$, and so $\hat{\sigma}^2 \sim \frac{\sigma^2}{n}\chi^2_{n-p}$.

(iii) $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}^2$ are independent.

The proof is not particularly elegant — it is just a whole lot of linear algebra!

Proof.

– We have $\hat{\boldsymbol{\beta}} = (X^TX)^{-1}X^T\mathbf{Y}$. Call this $C\mathbf{Y}$ for later use. Then $\hat{\boldsymbol{\beta}}$ has a normal distribution with mean

$$(X^TX)^{-1}X^T(X\boldsymbol{\beta}) = \boldsymbol{\beta}$$

and covariance

$$(X^TX)^{-1}X^T(\sigma^2 I)[(X^TX)^{-1}X^T]^T = \sigma^2(X^TX)^{-1}.$$

So

$$\hat{\boldsymbol{\beta}} \sim N_p(\boldsymbol{\beta}, \sigma^2(X^TX)^{-1}).$$

– Our previous lemma says that $\mathbf{Z}^TA\mathbf{Z} \sim \sigma^2\chi^2_r$. So we pick our $\mathbf{Z}$ and A so that $\mathbf{Z}^TA\mathbf{Z} = \text{RSS}$, and r, the degrees of freedom of A, is $n - p$.

Let $\mathbf{Z} = \mathbf{Y} - X\boldsymbol{\beta}$ and $A = (I_n - P)$, where $P = X(X^TX)^{-1}X^T$. We first check that the conditions of the lemma hold:

Since $\mathbf{Y} \sim N_n(X\boldsymbol{\beta}, \sigma^2 I)$, $\mathbf{Z} = \mathbf{Y} - X\boldsymbol{\beta} \sim N_n(\mathbf{0}, \sigma^2 I)$.

Since P is idempotent, $I_n - P$ also is (check!). We also have

$$\text{rank}(I_n - P) = \text{tr}(I_n - P) = n - p.$$

Therefore the conditions of the lemma hold.

To get the final useful result, we want to show that the RSS is indeed $\mathbf{Z}^TA\mathbf{Z}$. We simplify the expressions of RSS and $\mathbf{Z}^TA\mathbf{Z}$ and show that they are equal:

$$\mathbf{Z}^TA\mathbf{Z} = (\mathbf{Y} - X\boldsymbol{\beta})^T(I_n - P)(\mathbf{Y} - X\boldsymbol{\beta}) = \mathbf{Y}^T(I_n - P)\mathbf{Y}.$$

Noting the fact that $(I_n - P)X = \mathbf{0}$.

Writing $\mathbf{R} = \mathbf{Y} - \hat{\mathbf{Y}} = (I_n - P)\mathbf{Y}$, we have

$$\text{RSS} = \mathbf{R}^T\mathbf{R} = \mathbf{Y}^T(I_n - P)\mathbf{Y},$$

using the symmetry and idempotence of $I_n - P$.

Hence $\text{RSS} = \mathbf{Z}^TA\mathbf{Z} \sim \sigma^2\chi^2_{n-p}$. Then

$$\hat{\sigma}^2 = \frac{\text{RSS}}{n} \sim \frac{\sigma^2}{n}\chi^2_{n-p}.$$

– Let $V = \begin{pmatrix}\hat{\boldsymbol{\beta}} \\ \mathbf{R}\end{pmatrix} = D\mathbf{Y}$, where $D = \begin{pmatrix}C \\ I_n - P\end{pmatrix}$ is a $(p+n) \times n$ matrix.

Since $\mathbf{Y}$ is multivariate, V is multivariate with

$$\begin{aligned}
\text{cov}(V) &= D\sigma^2 I D^T \\
&= \sigma^2 \begin{pmatrix} CC^T & C(I_n - P)^T \\ (I_n - P)C^T & (I_n - P)(I_n - P)^T \end{pmatrix} \\
&= \sigma^2 \begin{pmatrix} CC^T & C(I_n - P) \\ (I_n - P)C^T & (I_n - P) \end{pmatrix} \\
&= \sigma^2 \begin{pmatrix} CC^T & 0 \\ 0 & I_n - P \end{pmatrix}
\end{aligned}$$

Using $C(I_n - P) = 0$ (since $(X^TX)^{-1}X^T(I_n - P) = 0$ since $(I_n - P)X = 0$ — check!).

Hence $\hat{\boldsymbol{\beta}}$ and $\mathbf{R}$ are independent since the off-diagonal covariant terms are 0. So $\hat{\boldsymbol{\beta}}$ and $\text{RSS} = \mathbf{R}^T\mathbf{R}$ are independent. So $\hat{\boldsymbol{\beta}}$ and $\hat{\sigma}^2$ are independent. □

From (ii), $\mathbb{E}(\text{RSS}) = \sigma^2(n-p)$. So $\tilde{\sigma}^2 = \frac{\text{RSS}}{n-p}$ is an unbiased estimator of σ^2. $\tilde{\sigma}$ is often known as the *residual standard error* on $n - p$ degrees of freedom.

3.4 The F distribution

Definition (F distribution)**.** Suppose U and V are independent with $U \sim \chi^2_m$ and $V \sim \chi^2_n$. The $X = \frac{U/m}{V/n}$ is said to have an *F-distribution* on m and n degrees of freedom. We write $X \sim F_{m,n}$

Since U and V have mean m and n respectively, U/m and V/n are approximately 1. So F is often approximately 1.

It should be very clear from definition that

Proposition. If $X \sim F_{m,n}$, then $1/X \sim F_{n,m}$.

We write $F_{m,n}(\alpha)$ be the upper $100\alpha\%$ point for the $F_{m,n}$-distribution so that if $X \sim F_{m,n}$, then $\mathbb{P}(X > F_{m,n}(\alpha)) = \alpha$.

Suppose that we have the upper 5% point for all $F_{n,m}$. Using these information, it is easy to find the *lower* 5% point for $F_{m,n}$ since we know that $\mathbb{P}(F_{m,n} < 1/x) = \mathbb{P}(F_{n,m} > x)$, which is where the above proposition comes useful.

Note that it is immediate from definitions of t_n and $F_{1,n}$ that if $Y \sim t_n$, then $Y^2 \sim F_{1,n}$, i.e. it is a ratio of independent χ^2_1 and χ^2_n variables.

3.5 Inference for $\boldsymbol{\beta}$

We know that $\hat{\boldsymbol{\beta}} \sim N_p(\boldsymbol{\beta}, \sigma^2(X^TX)^{-1})$. So

$$\hat{\beta}_j \sim N(\beta_j, \sigma^2(X^TX)^{-1}_{jj}).$$

The *standard error* of $\hat{\beta}_j$ is defined to be

$$\text{SE}(\hat{\beta}_j) = \sqrt{\tilde{\sigma}^2(X^TX)^{-1}_{jj}},$$

where $\tilde{\sigma}^2 = \text{RSS}/(n-p)$. Unlike the actual variance $\sigma^2(X^TX)^{-1}_{jj}$, the standard error is calculable from our data.

Then

$$\frac{\hat{\beta}_j - \beta_j}{\text{SE}(\hat{\beta}_j)} = \frac{\hat{\beta}_j - \beta_j}{\sqrt{\tilde{\sigma}^2(X^TX)^{-1}_{jj}}} = \frac{(\hat{\beta}_j - \beta_j)/\sqrt{\sigma^2(X^TX)^{-1}_{jj}}}{\sqrt{\text{RSS}/((n-p)\sigma^2)}}$$

By writing it in this somewhat weird form, we now recognize both the numerator and denominator. The numerator is a standard normal $N(0,1)$, and the

denominator is an independent $\sqrt{\chi^2_{n-p}/(n-p)}$, as we have previously shown. But a standard normal divided by χ^2 is, by definition, the t distribution. So

$$\frac{\hat{\beta}_j - \beta_j}{\mathrm{SE}(\hat{\beta}_j)} \sim t_{n-p}.$$

So a $100(1-\alpha)\%$ confidence interval for β_j has end points $\hat{\beta}_j \pm \mathrm{SE}(\hat{\beta}_j) t_{n-p}(\frac{\alpha}{2})$.

In particular, if we want to test $H_0 : \beta_j = 0$, we use the fact that under H_0, $\frac{\hat{\beta}_j}{\mathrm{SE}(\hat{\beta}_j)} \sim t_{n-p}$.

3.6 Simple linear regression

We can apply our results to the case of simple linear regression. We have

$$Y_i = a' + b(x_i - \bar{x}) + \varepsilon_i,$$

where $\bar{x} = \sum x_i/n$ and ε_i are iid $N(0, \sigma^2)$ for $i = 1, \cdots, n$.

Then we have

$$\begin{aligned}
\hat{a}' = \bar{Y} &\sim N\left(a', \frac{\sigma^2}{n}\right)\\
\hat{b} = \frac{S_{xY}}{S_{xx}} &\sim N\left(b, \frac{\sigma^2}{S_{xx}}\right)\\
\hat{Y}_i &= \hat{a}' + \hat{b}(x_i - \bar{x})\\
\mathrm{RSS} &= \sum_i (Y_i - \hat{Y}_i)^2 \sim \sigma^2 \chi^2_{n-2},
\end{aligned}$$

and $(\hat{a}', \hat{b})$ and $\hat{\sigma}^2 = \mathrm{RSS}/n$ are independent, as we have previously shown.

Note that $\hat{\sigma}^2$ is obtained by dividing RSS by n, and is the maximum likelihood estimator. On the other hand, $\tilde{\sigma}$ is obtained by dividing RSS by $n-p$, and is an unbiased estimator.

Example. Using the oxygen/time example, we have seen that

$$\tilde{\sigma}^2 = \frac{\mathrm{RSS}}{n-p} = \frac{67968}{24-2} = 3089 = 55.6^2.$$

So the standard error of $\hat{\beta}$ is

$$\mathrm{SE}(\hat{b}) = \sqrt{\tilde{\sigma}^2 (X^T X)^{-1}_{22}} = \sqrt{\frac{3089}{S_{xx}}} = \frac{55.6}{28.0} = 1.99.$$

So a 95% interval for b has end points

$$\hat{b} \pm \mathrm{SE}(\hat{b}) \times t_{n-p}(0.025) = 12.9 \pm 1.99 * t_{22}(0.025) = (-17.0, -8.8),$$

using the fact that $t_{22}(0.025) = 2.07$.

Note that this interval does not contain 0. So if we want to carry out a size 0.05 test of $H_0 : b = 0$ (they are uncorrelated) vs $H_1 : b \neq 0$ (they are correlated), the test statistic would be $\frac{\hat{b}}{\mathrm{SE}(\hat{b})} = \frac{-12.9}{1.99} = -6.48$. Then we reject H_0 because this is less than $-t_{22}(0.025) = -2.07$.

3.7 Expected response at $\mathbf{x}^*$

After performing the linear regression, we can now make *predictions* from it. Suppose that $\mathbf{x}^*$ is a new vector of values for the explanatory variables.

The expected response at $\mathbf{x}^*$ is $\mathbb{E}[\mathbf{Y} \mid \mathbf{x}^*] = \mathbf{x}^{*T}\boldsymbol{\beta}$. We estimate this by $\mathbf{x}^{*T}\hat{\boldsymbol{\beta}}$. Then we have

$$\mathbf{x}^{*T}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \sim N(0, \mathbf{x}^{*T}\operatorname{cov}(\hat{\boldsymbol{\beta}})\mathbf{x}^*) = N(0, \sigma^2\mathbf{x}^{*T}(X^TX)^{-1}\mathbf{x}^*).$$

Let $\tau^2 = \mathbf{x}^{*T}(X^TX)^{-1}\mathbf{x}^*$. Then

$$\frac{\mathbf{x}^{*T}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})}{\tilde{\sigma}\tau} \sim t_{n-p}.$$

Then a confidence interval for the expected response $\mathbf{x}^{*T}\boldsymbol{\beta}$ has end points

$$\mathbf{x}^{*T}\hat{\boldsymbol{\beta}} \pm \tilde{\sigma}\tau t_{n-p}\left(\frac{\alpha}{2}\right).$$

Example. Previous example continued:

Suppose we wish to estimate the time to run 2 miles for a man with an oxygen take-up measurement of 50. Here $\mathbf{x}^{*T} = (1, 50 - \bar{x})$, where $\bar{x} = 48.6$.

The estimated expected response at $\mathbf{x}^{*T}$ is

$$\mathbf{x}^{*T}\hat{\boldsymbol{\beta}} = \hat{a}' + (50 - 48.5) \times \hat{b} = 826.5 - 1.4 \times 12.9 = 808.5,$$

which is obtained by plugging $\mathbf{x}^{*T}$ into our fitted line.

We find

$$\tau^2 = \mathbf{x}^{*T}(X^TX)^{-1}\mathbf{x}^* = \frac{1}{n} + \frac{\mathbf{x}^{*2}}{S_{xx}} = \frac{1}{24} + \frac{1.4^2}{783.5} = 0.044 = 0.21^2.$$

So a 95% confidence interval for $\mathbb{E}[Y \mid \mathbf{x}^* = 50 - \bar{x}]$ is

$$\mathbf{x}^{*T}\hat{\boldsymbol{\beta}} \pm \tilde{\sigma}\tau t_{n-p}\left(\frac{\alpha}{2}\right) = 808.5 \pm 55.6 \times 0.21 \times 2.07 = (783.6, 832.2).$$

Note that this is the confidence interval for the predicted *expected value*, NOT the confidence interval for the actual obtained value.

The predicted response at $\mathbf{x}^*$ is $Y^* = \mathbf{x}^*\boldsymbol{\beta} + \varepsilon^*$, where $\varepsilon^* \sim N(0, \sigma^2)$, and Y^* is independent of $Y_1, \cdots, Y_n$. Here we have more uncertainties in our prediction: $\boldsymbol{\beta}$ and ε^*.

A $100(1-\alpha)\%$ *prediction interval* for Y^* is an interval $I(\mathbf{Y})$ such that $\mathbb{P}(Y^* \in I(\mathbf{Y})) = 1 - \alpha$, where the probability is over the joint distribution of $Y^*, Y_1, \cdots, Y_n$. So I is a random function of the past data $\mathbf{Y}$ that outputs an interval.

First of all, as above, the predicted *expected* response is $\hat{Y}^* = \mathbf{x}^{*T}\boldsymbol{\beta}$. This is an unbiased estimator since $\hat{Y}^* - Y^* = \mathbf{x}^{*T}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) - \varepsilon^*$, and hence

$$\mathbb{E}[\hat{Y}^* - Y^*] = \mathbf{x}^{*T}(\boldsymbol{\beta} - \boldsymbol{\beta}) = 0,$$

To find the variance, we use that fact that $\mathbf{x}^{*T}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})$ and ε^* are independent, and the variance of the sum of independent variables is the sum of the variances. So

$$\begin{aligned}\operatorname{var}(\hat{Y}^* - Y^*) &= \operatorname{var}(\mathbf{x}^{*T}(\hat{\boldsymbol{\beta}})) + \operatorname{var}(\varepsilon^*)\\ &= \sigma^2\mathbf{x}^{*T}(X^TX)^{-1}\mathbf{x}^* + \sigma^2.\\ &= \sigma^2(\tau^2 + 1).\end{aligned}$$

We can see this as the uncertainty in the regression line $\sigma^2\tau^2$, plus the wobble about the regression line σ^2. So

$$\hat{Y}^* - Y^* \sim N(0, \sigma^2(\tau^2 + 1)).$$

We therefore find that

$$\frac{\hat{Y}^* - Y^*}{\tilde{\sigma}\sqrt{\tau^2 + 1}} \sim t_{n-p}.$$

So the interval with endpoints

$$\mathbf{x}^{*T}\hat{\boldsymbol{\beta}} \pm \tilde{\sigma}\sqrt{\tau^2 + 1}t_{n-p}\left(\frac{\alpha}{2}\right)$$

is a 95% prediction interval for Y^*. We don't call this a confidence interval — confidence intervals are about finding parameters of the distribution, while the *prediction* interval is about our predictions.

Example. A 95% prediction interval for Y^* at $\mathbf{x}^{*T} = (1, (50 - \bar{x}))$ is

$$\mathbf{x}^{*T} \pm \tilde{\sigma}\sqrt{\tau^2 + 1}t_{n-p}\left(\frac{\alpha}{2}\right) = 808.5 \pm 55.6 \times 1.02 \times 2.07 = (691.1, 925.8).$$

Note that this is *much* wider than our our expected response! This is since there are three sources of uncertainty: we don't know what σ is, what $\hat{b}$ is, and the random ε fluctuation!

Example. Wafer example continued: Suppose we wish to estimate the expected resistivity of a new wafer in the first instrument. Here $\mathbf{x}^{*T} = (1, 0, \cdots, 0)$ (recall that $\mathbf{x}$ is an indicator vector to indicate which instrument is used).

The estimated response at $\mathbf{x}^{*T}$ is

$$\mathbf{x}^{*T}\hat{\boldsymbol{\mu}} = \hat{\mu}_1 = \bar{y_1} = 124.3$$

We find

$$\tau^2 = \mathbf{x}^{*T}(X^TX)^{-1}\mathbf{x}^* = \frac{1}{5}.$$

So a 95% confidence interval for $\mathbb{E}[Y_1^*]$ is

$$\mathbf{x}^{*T}\hat{\boldsymbol{\mu}} \pm \tilde{\sigma}\tau t_{n-p}\left(\frac{\alpha}{2}\right) = 124.3 \pm \frac{10.4}{\sqrt{5}} \times 2.09 = (114.6, 134.0).$$

Note that we are using an estimate of σ obtained from all five instruments. If we had only used the data from the first instrument, σ would be estimated as

$$\tilde{\sigma}_1 = \sqrt{\frac{\sum_{j=1}^{5} y_{1,j} - \bar{y_1}}{5 - 1}} = 8.74.$$

The observed 95% confidence interval for μ_1 would have been

$$\bar{y_1} \pm \frac{\tilde{\sigma}_1}{\sqrt{5}}t_4\left(\frac{\alpha}{2}\right) = 124.3 \pm 3.91 \times 2.78 = (113.5, 135.1),$$

which is *slightly* wider. Usually it is much wider, but in this special case, we only get little difference since the data from the first instrument is relatively tighter than the others.

A 95% prediction interval for Y_1^* at $\mathbf{x}^{*T} = (1, 0, \cdots, 0)$ is

$$\mathbf{x}^{*T}\hat{\boldsymbol{\mu}} \pm \tilde{\sigma}\sqrt{\tau^2 + 1}t_{n-p}\left(\frac{\alpha}{2}\right) = 124.3 \pm 10.42 \times 1.1 \times 2.07 = (100.5, 148.1).$$

3.8 Hypothesis testing

3.8.1 Hypothesis testing

In hypothesis testing, we want to know whether certain variables influence the result. If, say, the variable x_1 does not influence Y, then we must have $\beta_1 = 0$. So the goal is to test the hypothesis $H_0 : \beta_1 = 0$ versus $H_1 : \beta_1 \neq 0$. We will tackle a more general case, where $\boldsymbol{\beta}$ can be split into two vectors $\boldsymbol{\beta}_0$ and $\boldsymbol{\beta}_1$, and we test if $\boldsymbol{\beta}_1$ is zero.

We start with an obscure lemma, which might seem pointless at first, but will prove itself useful very soon.

Lemma. Suppose $\mathbf{Z} \sim N_n(\mathbf{0}, \sigma^2 I_n)$, and A_1 and A_2 are symmetric, idempotent $n \times n$ matrices with $A_1 A_2 = 0$ (i.e. they are orthogonal). Then $\mathbf{Z}^T A_1 \mathbf{Z}$ and $\mathbf{Z}^T A_2 \mathbf{Z}$ are independent.

This is geometrically intuitive, because A_1 and A_2 being orthogonal means they are concerned about different parts of the vector $\mathbf{Z}$.

Proof. Let $\mathbf{X}_i = A_i \mathbf{Z}$, $i = 1, 2$ and

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}_1 \\ \mathbf{W}_2 \end{pmatrix} = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} \mathbf{Z}.$$

Then

$$\mathbf{W} \sim N_{2n}\left(\begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \sigma^2 \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} \right)$$

since the off diagonal matrices are $\sigma^2 A_1^T A_2 = A_1 A_2 = 0$.

So $\mathbf{W}_1$ and $\mathbf{W}_2$ are independent, which implies

$$\mathbf{W}_1^T \mathbf{W}_1 = \mathbf{Z}^T A_1^T A_1 \mathbf{Z} = \mathbf{Z}^T A_1 A_1 \mathbf{Z} = \mathbf{Z}^T A_1 \mathbf{Z}$$

and

$$\mathbf{W}_2^T \mathbf{W}_2 = \mathbf{Z}^T A_2^T A_2 \mathbf{Z} = \mathbf{Z}^T A_2 A_2 \mathbf{Z} = \mathbf{Z}^T A_2 \mathbf{Z}$$

are independent □

Now we go to hypothesis testing in general linear models:

Suppose $\underset{n \times p}{X} = \begin{pmatrix} \underset{n \times p_0}{X_0} & \underset{n \times (p - p_0)}{X_1} \end{pmatrix}$ and $\mathbf{B} = \begin{pmatrix} \boldsymbol{\beta}_0 \\ \boldsymbol{\beta}_1 \end{pmatrix}$, where $\operatorname{rank}(X) = p, \operatorname{rank}(X_0) = p_0$.

We want to test $H_0 : \boldsymbol{\beta}_1 = 0$ against $H_1 : \boldsymbol{\beta}_1 \neq 0$. Under H_0, $X_1 \boldsymbol{\beta}_1$ vanishes and

$$\mathbf{Y} = X_0 \boldsymbol{\beta} + \boldsymbol{\varepsilon}.$$

Under H_0, the mle of $\boldsymbol{\beta}_0$ and σ^2 are

$$\begin{aligned} \hat{\hat{\boldsymbol{\beta}}}_0 &= (X_0^T X_0)^{-1} X_0^T \mathbf{Y} \\ \hat{\hat{\sigma}}^2 &= \frac{\mathrm{RSS}_0}{n} = \frac{1}{n} (\mathbf{Y} - X_0 \hat{\hat{\boldsymbol{\beta}}}_0)^T (\mathbf{Y} - X_0 \hat{\hat{\boldsymbol{\beta}}}_0) \end{aligned}$$

and we have previously shown these are independent.

Note that our poor estimators wear two hats instead of one. We adopt the convention that the estimators of the null hypothesis have two hats, while those of the alternative hypothesis have one.

So the fitted values under H_0 are

$$\hat{\hat{\mathbf{Y}}} = X_0(X_0^T X_0)^{-1} X_0^T \mathbf{Y} = P_0 \mathbf{Y},$$

where $P_0 = X_0(X_0^T X_0)^{-1} X_0^T$.

The generalized likelihood ratio test of H_0 against H_1 is

$$\begin{aligned}
\Lambda_{\mathbf{Y}}(H_0, H_1) &= \frac{\left(\frac{1}{\sqrt{2\pi\hat{\sigma}^2}}\right) \exp\left(-\frac{1}{2\hat{\sigma}^2}(\mathbf{Y} - X\hat{\boldsymbol{\beta}})^T(\mathbf{Y} - X\hat{\boldsymbol{\beta}})\right)}{\left(\frac{1}{\sqrt{2\pi\hat{\sigma}^2}}\right) \exp\left(-\frac{1}{2\hat{\sigma}^2}(\mathbf{Y} - X\hat{\hat{\boldsymbol{\beta}}}_0)^T(\mathbf{Y} - X\hat{\hat{\boldsymbol{\beta}}}_0)\right)} \\
&= \left(\frac{\hat{\hat{\sigma}}^2}{\hat{\sigma}^2}\right)^{n/2} \\
&= \left(\frac{\mathrm{RSS}_0}{\mathrm{RSS}}\right)^{n/2} \\
&= \left(1 + \frac{\mathrm{RSS}_0 - \mathrm{RSS}}{\mathrm{RSS}}\right)^{n/2}.
\end{aligned}$$

We reject H_0 when $2\log\Lambda$ is large, equivalently when $\frac{\mathrm{RSS}_0 - \mathrm{RSS}}{\mathrm{RSS}}$ is large.

Using the results in Lecture 8, under H_0, we have

$$2\log\Lambda = n\log\left(1 + \frac{\mathrm{RSS}_0 - \mathrm{RSS}}{\mathrm{RSS}}\right),$$

which is approximately a $\chi^2_{p_1 - p_0}$ random variable.

This is a good approximation. But we can get an exact null distribution, and get an exact test.

We have previously shown that $\mathrm{RSS} = \mathbf{Y}^T(I_n - P)\mathbf{Y}$, and so

$$\mathrm{RSS}_0 - \mathrm{RSS} = \mathbf{Y}^T(I_n - P_0)\mathbf{Y} - \mathbf{Y}^T(I_n - P)\mathbf{Y} = \mathbf{Y}^T(P - P_0)\mathbf{Y}.$$

Now both $I_n - P$ and $P - P_0$ are symmetric and idempotent, and therefore $\mathrm{rank}(I_n - P) = n - p$ and

$$\mathrm{rank}(P - P_0) = \mathrm{tr}(P - P_0) = \mathrm{tr}(P) - \mathrm{tr}(P_0) = \mathrm{rank}(P) - \mathrm{rank}(P_0) = p - p_0.$$

Also,

$$(I_n - P)(P - P_0) = (I_n - P)P - (I_n - P)P_0 = (P - P^2) - (P_0 - PP_0) = 0.$$

(we have $P^2 = P$ by idempotence, and $PP_0 = P_0$ since after projecting with P_0, we are already in the space of P, and applying P has no effect)

Finally,

$$\begin{aligned}
\mathbf{Y}^T(I_n - P)\mathbf{Y} &= (\mathbf{Y} - X_0\boldsymbol{\beta}_0)^T(I_n - P)(\mathbf{Y} - X_0\boldsymbol{\beta}_0) \\
\mathbf{Y}^T(P - P_0)\mathbf{Y} &= (\mathbf{Y} - X_0\boldsymbol{\beta}_0)^T(P - P_0)(\mathbf{Y} - X_0\boldsymbol{\beta}_0)
\end{aligned}$$

since $(I_n - P)X_0 = (P - P_0)X_0 = 0$.

If we let $\mathbf{Z} = \mathbf{Y} - X_0\boldsymbol{\beta}_0$, $A_1 = I_n - P$, $A_2 = P - P_0$, and apply our previous lemma, and the fact that $\mathbf{Z}^T A_i \mathbf{Z} \sim \sigma^2 \chi^2_r$, then

$$\text{RSS} = \mathbf{Y}^T(I_n - P)\mathbf{Y} \sim \chi^2_{n-p}$$
$$\text{RSS}_0 - \text{RSS} = \mathbf{Y}^T(P - P_0)\mathbf{Y} \sim \chi^2_{p-p_0}$$

and these random variables are independent.

So under H_0,

$$F = \frac{\mathbf{Y}^T(P - P_0)\mathbf{Y}/(p - p_0)}{\mathbf{Y}^T(I_n - P)\mathbf{Y}/(n - p)} = \frac{(\text{RSS}_0 - \text{RSS})/(p - p_0)}{\text{RSS}/(n - p)} \sim F_{p-p_0, n-p},$$

Hence we reject H_0 if $F > F_{p-p_0,n-p}(\alpha)$.

$\text{RSS}_0 - \text{RSS}$ is the reduction in the sum of squares due to fitting $\boldsymbol{\beta}_1$ in addition to $\boldsymbol{\beta}_0$.

Source of var.	d.f.	sum of squares	mean squares	F statistic
Fitted model	$p - p_0$	$\text{RSS}_0 - \text{RSS}$	$\frac{\text{RSS}_0 - \text{RSS}}{p-p_0}$	$\frac{(\text{RSS}_0 - \text{RSS})/(p-p_0)}{\text{RSS}/(n-p)}$
Residual	$n - p$	RSS	$\frac{\text{RSS}}{n-p}$	
Total	$n - p_0$	RSS_0		

The ratio $\frac{\text{RSS}_0 - \text{RSS}}{\text{RSS}_0}$ is sometimes known as the *proportion of variance explained* by $\boldsymbol{\beta}_1$, and denoted R^2.

3.8.2 Simple linear regression

We assume that

$$Y_i = a' + b(x_i - \bar{x}) + \varepsilon_i,$$

where $\bar{x} = \sum x_i/n$ and ε_i are $N(0, \sigma^2)$.

Suppose we want to test the hypothesis $H_0 : b = 0$, i.e. no linear relationship. We have previously seen how to construct a confidence interval, and so we could simply see if it included 0.

Alternatively, under H_0, the model is $Y_i \sim N(a', \sigma^2)$, and so $\hat{a}' = \bar{Y}$, and the fitted values are $\hat{Y}_i = \bar{Y}$.

The observed RSS_0 is therefore

$$\text{RSS}_0 = \sum_i (y_i - \bar{y})^2 = S_{yy}.$$

The fitted sum of squares is therefore

$$\text{RSS}_0 - \text{RSS} = \sum_i \left((y_i - \bar{y})^2 - (y_i - \bar{y} - \hat{b}(x_i - \bar{x}))^2\right) = \hat{b}^2 \sum (x_i - \bar{x})^2 = \hat{b}^2 S_{xx}.$$

Source of var.	d.f.	sum of squares	mean squares	F statistic
Fitted model	1	$\text{RSS}_0 - \text{RSS} = \hat{b}^2 S_{XX}$	$\hat{b}^2 S_{xx}$	$F = \frac{\hat{b}^2 S_{xx}}{\tilde{\sigma}^2}$
Residual	$n - 2$	$\text{RSS} = \sum_i (y_i - \hat{y})^2$	$\tilde{\sigma}^2$.	
Total	$n - 1$	$\text{RSS}_0 = \sum_i (y_i - \bar{y})^2$		

Note that the proposition of variance explained is $\hat{b}^2 S_{xx}/S_{yy} = \frac{S_{xy}^2}{S_{xx}S_{yy}} = r^2$, where r is the Pearson's product-moment correlation coefficient

$$r = \frac{S_{xy}}{\sqrt{S_{xx}S_{yy}}}.$$

We have previously seen that under H_0, $\frac{\hat{b}}{\mathrm{SE}(\hat{b})} \sim t_{n-2}$, where $\mathrm{SE}(\hat{b}) = \tilde{\sigma}/\sqrt{S_{xx}}$. So we let

$$t = \frac{\hat{b}}{\mathrm{SE}(\hat{b})} = \frac{\hat{b}\sqrt{S_{xx}}}{\tilde{\sigma}}.$$

Checking whether $|t| > t_{n-2}\left(\frac{\alpha}{2}\right)$ is precisely the same as checking whether $t^2 = F > F_{1,n-2}(\alpha)$, since a $F_{1,n-2}$ variable is t_{n-2}^2.

Hence the same conclusion is reached, regardless of whether we use the t-distribution or the F statistic derived form an analysis of variance table.

3.8.3 One way analysis of variance with equal numbers in each group

Recall that in our wafer example, we made measurements in groups, and want to know if there is a difference between groups. In general, suppose J measurements are taken in each of I groups, and that

$$Y_{ij} = \mu_i + \varepsilon_{ij},$$

where ε_{ij} are independent $N(0, \sigma^2)$ random variables, and the μ_i are unknown constants.

Fitting this model gives

$$\mathrm{RSS} = \sum_{i=1}^{I}\sum_{j=1}^{J}(Y_{ij} - \hat{\mu}_i)^2 = \sum_{i=1}^{I}\sum_{j=1}^{J}(Y_{ij} - \bar{Y}_{i.})^2$$

on $n - I$ degrees of freedom.

Suppose we want to test the hypothesis $H_0 : \mu_i = \mu$, i.e. no difference between groups.

Under H_0, the model is $Y_{ij} \sim N(\mu, \sigma^2)$, and so $\hat{\mu} = \bar{Y}$, and the fitted values are $\hat{Y_{ij}} = \bar{Y}$.

The observed RSS_0 is therefore

$$\mathrm{RSS}_0 = \sum_{i,j}(y_{ij} - \bar{y}_{..})^2.$$

The fitted sum of squares is therefore

$$\mathrm{RSS}_0 - \mathrm{RSS} = \sum_i\sum_j\left((y_{ij} - \bar{y}_{..})^2 - (y_{ij} - \bar{y}_{i.})^2\right) = J\sum_i(\bar{y}_{i.} - \bar{y}_{..})^2.$$

Source of var.	d.f.	sum of squares	mean squares	F statistic
Fitted model	$I-1$	$J\sum_i(\bar{y}_i - \bar{y}_{..})^2$	$J\sum_i \frac{(\bar{y}_{i.}-\bar{y}_{..})^2}{I-1}$	$J\sum_i \frac{(\bar{y}_{i.}-\bar{y}_{..})^2}{(I-1)\tilde{\sigma}^2}$
Residual	$n-I$	$\sum_i\sum_j(y_{ij} - \bar{y}_{i.})^2$	$\tilde{\sigma}^2$	
Total	$n-1$	$\sum_i\sum_j(y_{ij} - \bar{y}_{..})^2$		